Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:49 PM GMT

PDB ID	:	4PZD
Title	:	Crystal structure of (S)-3-hydroxybutyryl-CoA dehydrogenase PaaH1 in complex with NAD+
Authors	:	Kim, J.; Chang, J.H.; Kim, K.J.
Deposited on	:	2014-03-29
Resolution	:	2.61 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:

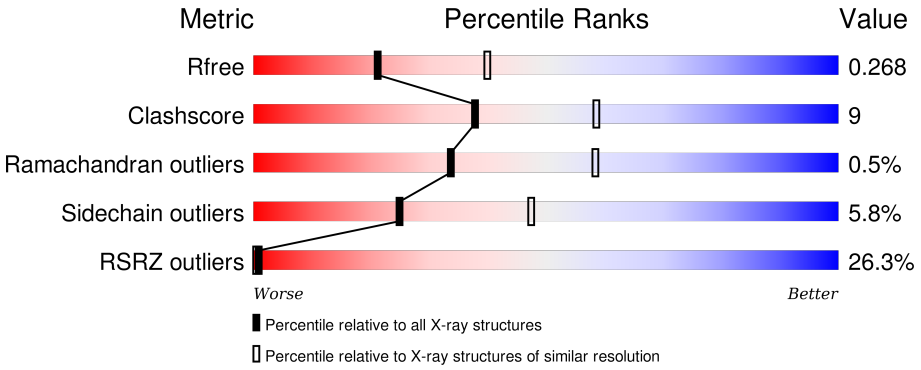
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.61 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	284	28% 77% 20%
1	B	284	27% 78% 20%
1	C	284	13% 79% 19%
1	D	284	35% 77% 21%
1	E	284	31% 79% 20%

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Mol	Chain	Length	Quality of chain
1	F	284	16% 82% 16%
1	G	284	37% 82% 16%
1	H	284	32% 76% 21%
1	I	284	18% 83% 16%

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	NAD	C	301	-	-	-	X
2	NAD	E	301	-	-	-	X
2	NAD	G	301	-	-	-	X
2	NAD	I	301	-	-	-	X

2 Entry composition (i)

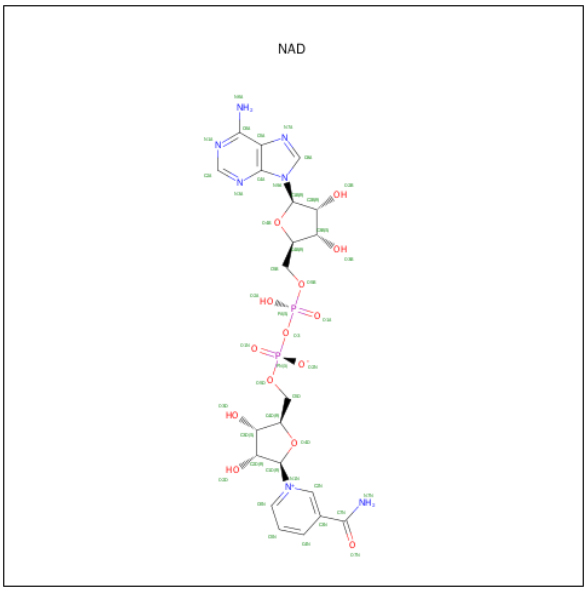
There are 3 unique types of molecules in this entry. The entry contains 19415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-Hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	B	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	C	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	D	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	E	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	F	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	G	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	H	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			
1	I	283	Total	C	N	O	S	0	0	0
			2102	1331	355	400	16			

- 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		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	10	Total	O	0	0
			10	10		
3	C	17	Total	O	0	0
			17	17		

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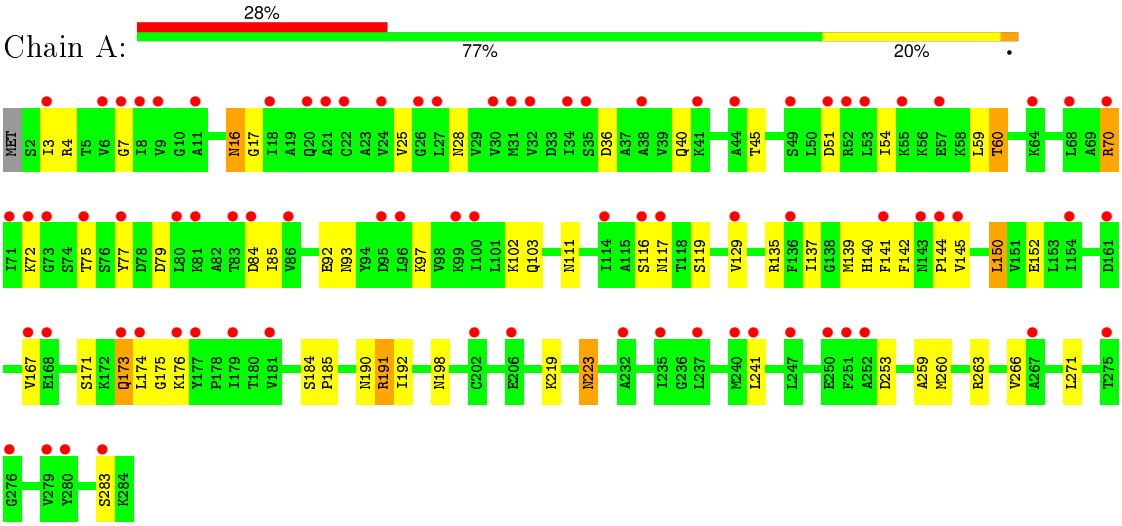
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	6	Total O 6 6	0	0
3	E	14	Total O 14 14	0	0
3	F	17	Total O 17 17	0	0
3	G	7	Total O 7 7	0	0
3	H	9	Total O 9 9	0	0
3	I	11	Total O 11 11	0	0

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.

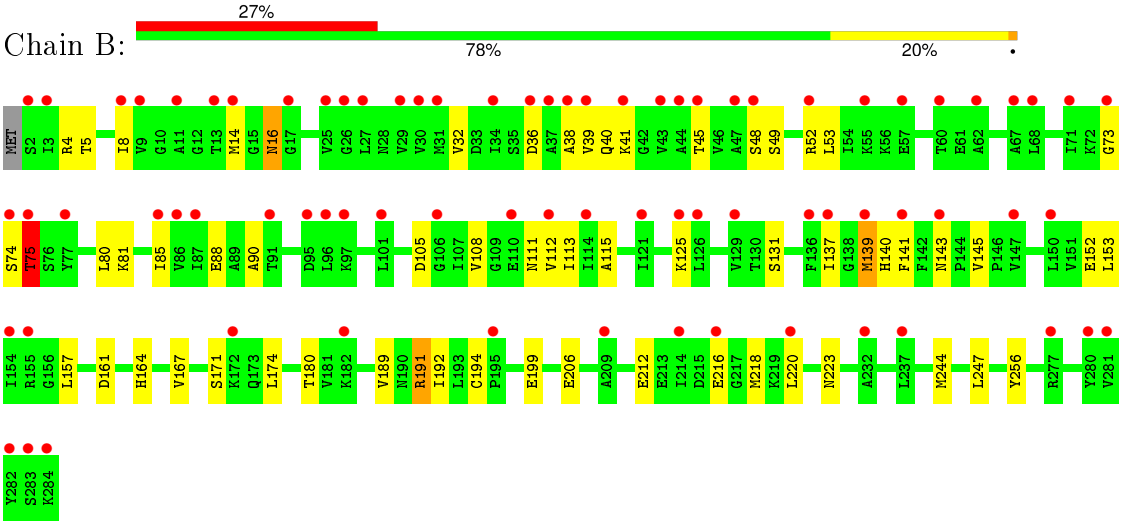
- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

Chain A:



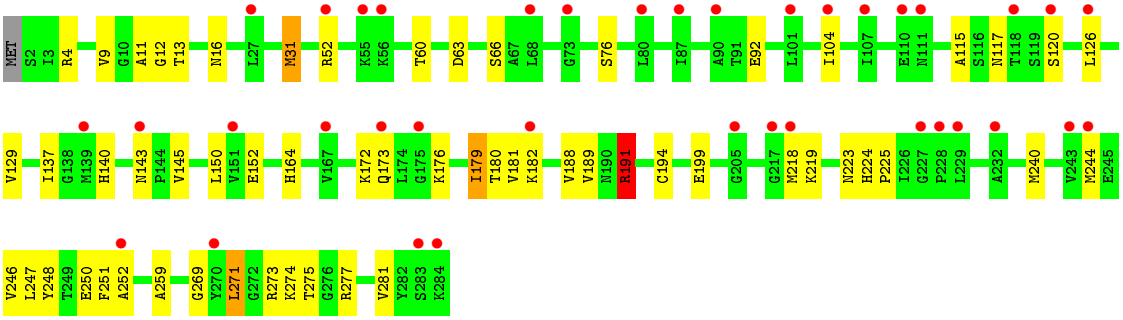
- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

Chain B:



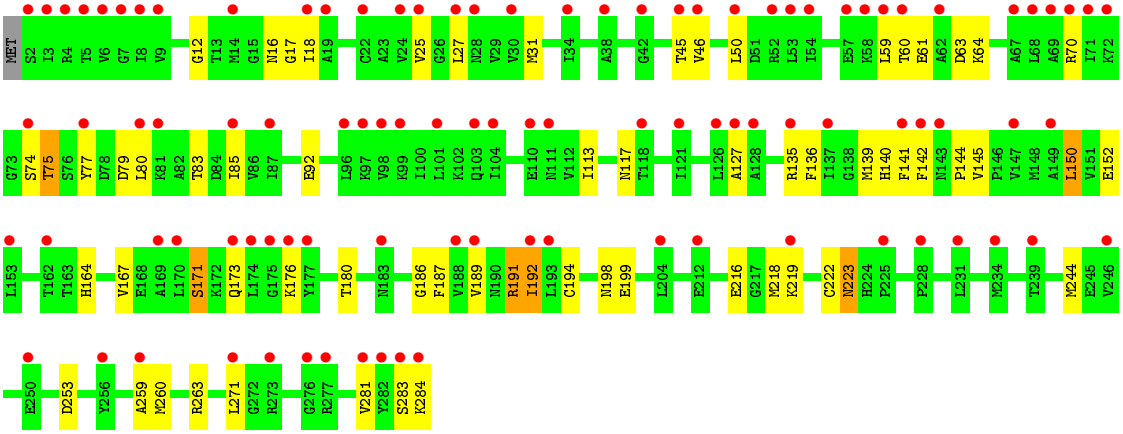
- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

Chain C:



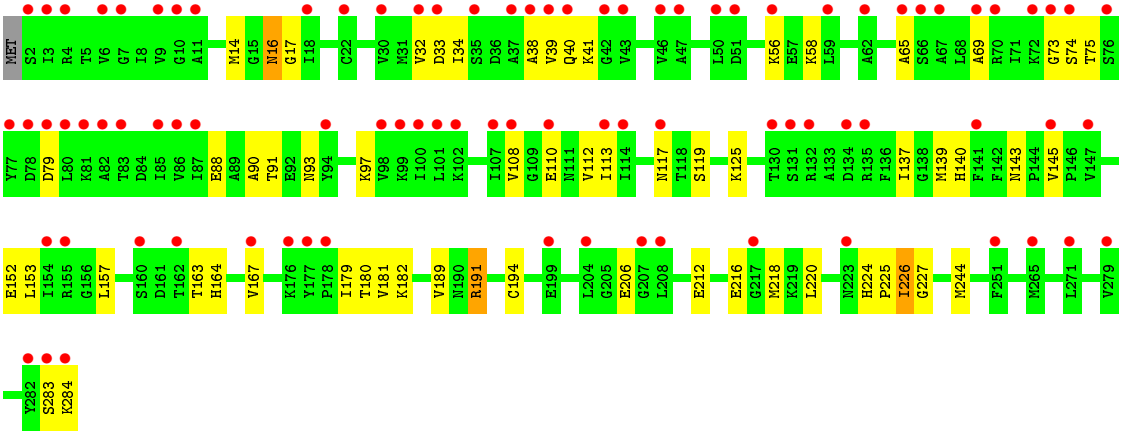
• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

Chain D:



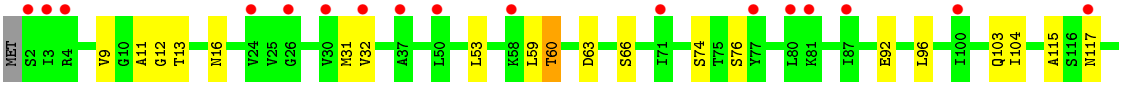
• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

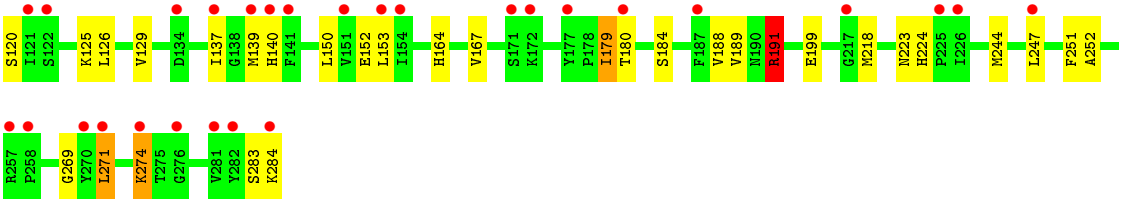
Chain E:



• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

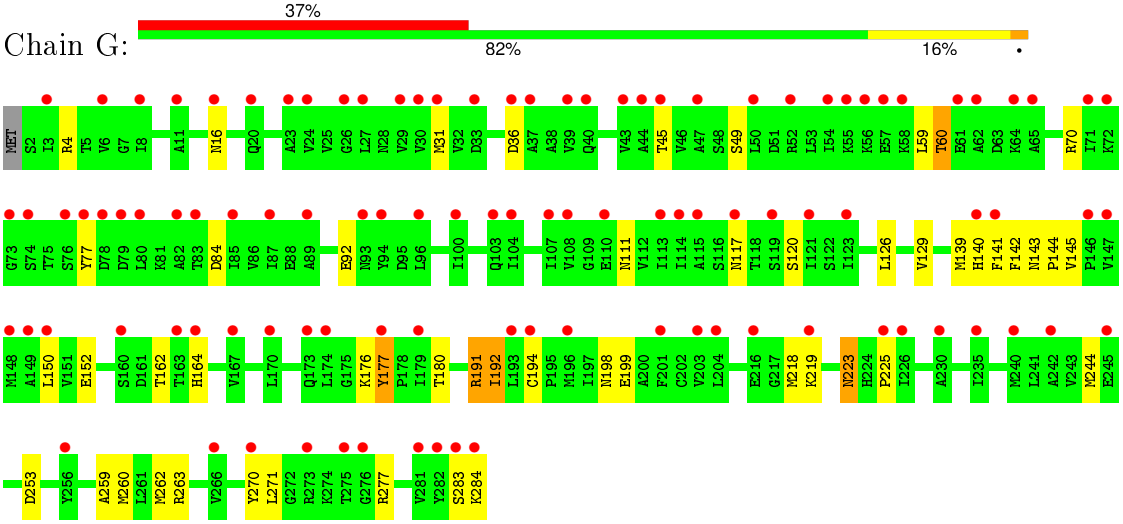
Chain F:





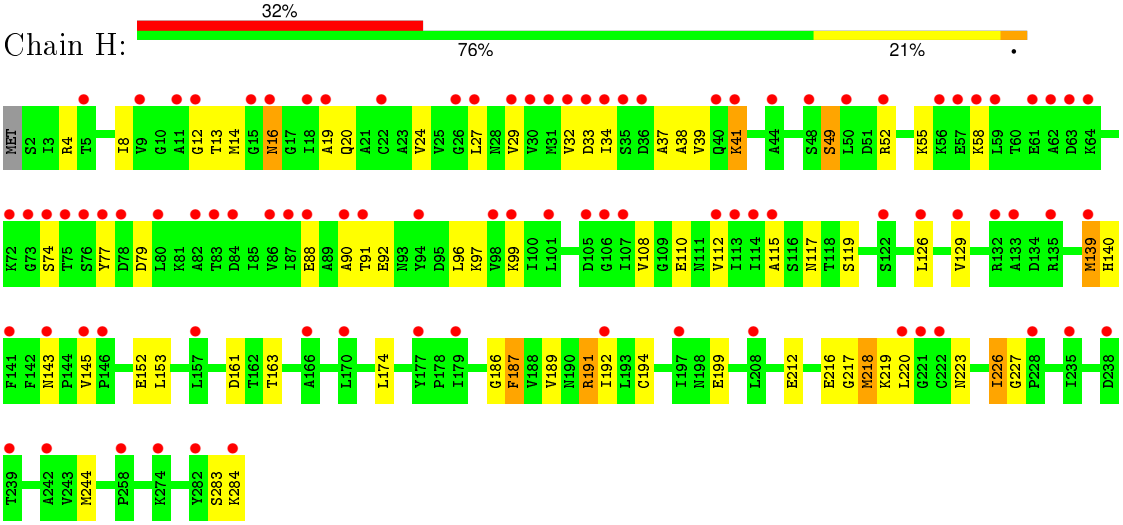
• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

Chain G:



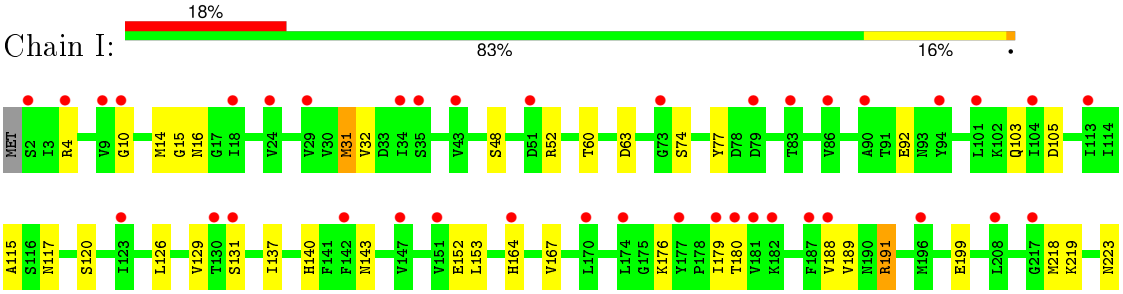
• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

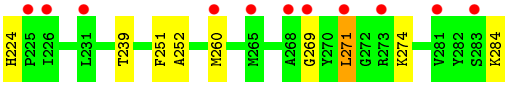
Chain H:



• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

Chain I:




H224
P225
T226
L231
T239
F251
A252
M260
M265
A268
G269
Y270
L271
G272
R273
K274
Y281
Y282
S283
K284

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.08Å 135.59Å 97.44Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 32.85 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.61) 98.6 (32.85-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.02 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.199 , 0.269 0.199 , 0.268	Depositor DCC
R_{free} test set	4557 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.6	EDS
Estimated twinning fraction	0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.013 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.439 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.437 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.013 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 91442 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19415	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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	0.59	0/2128	0.81	3/2879 (0.1%)
1	B	0.60	0/2128	0.78	2/2879 (0.1%)
1	C	0.67	0/2128	0.79	1/2879 (0.0%)
1	D	0.59	0/2128	0.82	4/2879 (0.1%)
1	E	0.58	0/2128	0.78	0/2879
1	F	0.68	0/2128	0.85	4/2879 (0.1%)
1	G	0.60	0/2128	0.81	4/2879 (0.1%)
1	H	0.59	0/2128	0.77	2/2879 (0.1%)
1	I	0.68	0/2128	0.82	1/2879 (0.0%)
All	All	0.62	0/19152	0.81	21/25911 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	G	0	1
All	All	0	5

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	75	THR	CB-CA-C	8.98	135.84	111.60
1	A	253	ASP	CB-CG-OD1	8.57	126.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	184	SER	CB-CA-C	7.86	125.03	110.10
1	G	253	ASP	CB-CG-OD1	7.56	125.10	118.30
1	F	191	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	F	191	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	G	191	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	191	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	D	253	ASP	CB-CG-OD1	6.65	124.28	118.30
1	H	187	PHE	N-CA-C	-6.06	94.63	111.00
1	B	75	THR	C-N-CA	5.71	135.98	121.70
1	F	191	ARG	CG-CD-NE	-5.70	99.83	111.80
1	A	253	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	I	31	MET	CG-SD-CE	-5.33	91.68	100.20
1	G	191	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	31	MET	CG-SD-CE	-5.25	91.81	100.20
1	H	218	MET	CG-SD-CE	-5.21	91.86	100.20
1	D	253	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	191	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	G	253	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	D	191	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	PHE	Peptide
1	B	75	THR	Peptide
1	C	191	ARG	Sidechain
1	D	142	PHE	Peptide
1	G	142	PHE	Peptide

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	2102	0	2187	32	0
1	B	2102	0	2187	42	0
1	C	2102	0	2187	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2102	0	2187	51	0
1	E	2102	0	2187	42	0
1	F	2102	0	2187	38	0
1	G	2102	0	2187	41	0
1	H	2102	0	2187	54	0
1	I	2102	0	2187	43	0
2	A	44	0	26	3	0
2	B	44	0	26	0	0
2	C	44	0	26	4	0
2	D	44	0	26	6	0
2	E	44	0	26	2	0
2	F	44	0	26	4	0
2	G	44	0	26	5	0
2	H	44	0	26	5	0
2	I	44	0	26	7	0
3	A	10	0	0	4	0
3	B	10	0	0	3	0
3	C	17	0	0	6	0
3	D	6	0	0	3	0
3	E	14	0	0	5	0
3	F	17	0	0	1	0
3	G	7	0	0	1	0
3	H	9	0	0	6	0
3	I	11	0	0	6	0
All	All	19415	0	19917	360	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 9.

All (360) 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:B:32:VAL:HG13	1:B:75:THR:O	1.56	1.04
1:F:244:MET:HE2	1:F:247:LEU:HD12	1.41	1.02
1:B:14:MET:SD	1:B:143:ASN:ND2	2.36	0.98
1:E:14:MET:SD	1:E:143:ASN:ND2	2.43	0.90
1:H:14:MET:SD	1:H:143:ASN:ND2	2.46	0.89
1:B:32:VAL:CG1	1:B:75:THR:O	2.23	0.86
1:F:244:MET:CE	1:F:247:LEU:HD12	2.05	0.85
1:C:244:MET:HE2	1:C:247:LEU:HD12	1.59	0.84
1:D:198:ASN:HD21	1:D:259:ALA:H	1.23	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:CYS:HB3	1:E:244:MET:CE	2.10	0.81
1:I:16:ASN:HA	1:I:31:MET:HE3	1.64	0.80
1:C:92:GLU:HG2	2:C:301:NAD:O2D	1.82	0.80
1:H:37:ALA:HB1	3:H:409:HOH:O	1.82	0.79
1:I:52:ARG:HD3	3:I:407:HOH:O	1.84	0.77
1:C:16:ASN:HA	1:C:31:MET:HE3	1.68	0.76
1:B:191:ARG:NH1	1:C:199:GLU:OE2	2.20	0.75
1:A:198:ASN:HD21	1:A:259:ALA:H	1.36	0.74
1:H:39:VAL:HG21	1:H:74:SER:O	1.88	0.74
1:A:92:GLU:HG2	2:A:301:NAD:H2D	1.69	0.74
1:E:191:ARG:NH1	1:F:199:GLU:OE2	2.22	0.73
1:I:152:GLU:HA	1:I:179:ILE:HG22	1.71	0.72
1:H:108:VAL:HG11	1:H:112:VAL:HG11	1.71	0.72
1:E:16:ASN:C	1:E:16:ASN:HD22	1.92	0.72
1:H:194:CYS:HB3	1:H:244:MET:HE3	1.72	0.72
1:G:117:ASN:HD21	1:G:141:PHE:H	1.37	0.72
1:G:198:ASN:HD21	1:G:259:ALA:H	1.36	0.71
1:H:88:GLU:OE1	1:H:97:LYS:NZ	2.22	0.71
1:H:192:ILE:HD12	1:I:218:MET:HE3	1.71	0.71
1:H:8:ILE:HG22	1:H:8:ILE:O	1.90	0.70
1:D:199:GLU:HB3	1:G:192:ILE:HG22	1.74	0.70
1:B:39:VAL:HG21	1:B:74:SER:O	1.91	0.70
1:A:145:VAL:O	1:A:176:LYS:NZ	2.26	0.69
1:H:34:ILE:HG22	3:H:408:HOH:O	1.91	0.69
1:I:60:THR:HG23	1:I:63:ASP:H	1.56	0.69
1:B:194:CYS:HB3	1:B:244:MET:HE3	1.76	0.68
1:I:143:ASN:HB2	3:I:408:HOH:O	1.92	0.68
1:I:117:ASN:HD21	2:I:301:NAD:H6N	1.59	0.67
1:H:79:ASP:HB2	3:H:406:HOH:O	1.94	0.67
1:A:92:GLU:HG2	2:A:301:NAD:C2D	2.24	0.66
1:A:117:ASN:HD21	1:A:141:PHE:H	1.42	0.66
1:D:260:MET:CE	3:D:403:HOH:O	2.43	0.66
1:H:38:ALA:HA	1:H:41:LYS:HE3	1.77	0.66
1:C:52:ARG:HD3	3:C:413:HOH:O	1.94	0.66
1:H:191:ARG:NH1	1:I:199:GLU:OE2	2.30	0.65
1:D:194:CYS:HB3	1:D:244:MET:HE3	1.78	0.65
1:E:108:VAL:HG11	1:E:112:VAL:HG11	1.79	0.65
1:D:117:ASN:HA	1:D:139:MET:O	1.97	0.65
1:C:244:MET:CE	1:C:247:LEU:HD12	2.27	0.63
1:D:199:GLU:CG	1:G:192:ILE:HG22	2.28	0.63
1:G:145:VAL:O	1:G:176:LYS:NZ	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:ASN:CB	3:I:408:HOH:O	2.45	0.62
1:B:192:ILE:HD12	1:C:218:MET:HE3	1.81	0.62
1:B:108:VAL:HG11	1:B:112:VAL:HG11	1.81	0.62
1:B:191:ARG:HD3	3:B:404:HOH:O	1.98	0.62
1:D:218:MET:CE	1:D:222:CYS:SG	2.87	0.62
1:I:117:ASN:ND2	2:I:301:NAD:H1D	2.14	0.61
1:A:4:ARG:N	1:A:84:ASP:OD2	2.34	0.61
1:F:16:ASN:HA	1:F:31:MET:HE3	1.81	0.61
1:A:260:MET:HE1	3:A:402:HOH:O	1.99	0.61
1:F:92:GLU:HG2	2:F:301:NAD:O2D	2.01	0.61
1:C:117:ASN:HD21	2:C:301:NAD:H6N	1.66	0.61
1:B:38:ALA:HA	1:B:41:LYS:HG2	1.82	0.60
1:D:117:ASN:HD21	1:D:141:PHE:H	1.48	0.60
1:H:194:CYS:HB3	1:H:244:MET:CE	2.32	0.60
1:F:92:GLU:HG2	2:F:301:NAD:C2D	2.32	0.60
1:E:194:CYS:HB3	1:E:244:MET:HE1	1.84	0.60
1:A:260:MET:CE	3:A:402:HOH:O	2.50	0.60
1:C:143:ASN:HA	3:C:404:HOH:O	2.02	0.59
1:E:39:VAL:HG21	1:E:74:SER:O	2.02	0.59
1:D:18:ILE:HD13	1:D:145:VAL:HG11	1.84	0.59
1:D:189:VAL:HA	1:G:218:MET:CE	2.33	0.59
1:F:76:SER:HB3	3:F:413:HOH:O	2.03	0.59
1:H:199:GLU:OE2	1:I:191:ARG:NH1	2.34	0.58
1:C:251:PHE:O	1:C:252:ALA:HB3	2.02	0.58
1:I:219:LYS:O	1:I:223:ASN:HA	2.04	0.58
1:G:140:HIS:HB3	1:G:152:GLU:HB2	1.85	0.58
1:D:199:GLU:CB	1:G:192:ILE:HG22	2.33	0.58
1:E:73:GLY:HA3	3:E:408:HOH:O	2.04	0.58
1:B:32:VAL:HG13	1:B:75:THR:C	2.23	0.57
1:I:251:PHE:O	1:I:252:ALA:HB3	2.03	0.57
1:B:88:GLU:OE2	1:B:90:ALA:N	2.38	0.57
1:A:77:TYR:HB3	3:A:410:HOH:O	2.04	0.57
1:D:164:HIS:HE1	1:D:180:THR:OG1	1.88	0.57
1:E:140:HIS:HB3	1:E:152:GLU:HB2	1.87	0.57
1:C:60:THR:HG21	3:C:407:HOH:O	2.04	0.56
1:H:189:VAL:HA	1:I:218:MET:CE	2.35	0.56
1:E:79:ASP:HB2	3:E:413:HOH:O	2.05	0.56
1:B:113:ILE:HD11	3:B:406:HOH:O	2.05	0.56
1:I:199:GLU:HA	1:I:199:GLU:OE1	2.05	0.56
1:B:140:HIS:HB3	1:B:152:GLU:HB2	1.88	0.56
1:D:59:LEU:HB3	1:D:60:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:ALA:HA	1:H:41:LYS:CE	2.36	0.56
1:F:152:GLU:HA	1:F:179:ILE:HG23	1.86	0.56
1:D:219:LYS:HE2	3:D:406:HOH:O	2.06	0.56
1:G:194:CYS:O	1:G:244:MET:HE3	2.06	0.56
1:G:77:TYR:OH	2:G:301:NAD:N1A	2.39	0.55
1:C:164:HIS:HE1	1:C:180:THR:OG1	1.88	0.55
1:B:218:MET:CE	1:C:189:VAL:HA	2.37	0.55
1:F:251:PHE:O	1:F:252:ALA:HB3	2.05	0.55
1:C:126:LEU:O	1:C:129:VAL:HG22	2.06	0.55
1:B:223:ASN:HB2	1:C:225:PRO:HG3	1.89	0.55
1:E:16:ASN:HD22	1:E:17:GLY:N	2.03	0.55
1:E:194:CYS:HB3	1:E:244:MET:HE3	1.87	0.55
1:C:269:GLY:C	1:C:271:LEU:HD13	2.26	0.55
1:I:92:GLU:HG2	2:I:301:NAD:C2D	2.36	0.55
1:D:218:MET:CE	1:D:218:MET:HA	2.37	0.55
1:D:216:GLU:OE1	1:G:177:TYR:CE1	2.59	0.55
1:D:189:VAL:HA	1:G:218:MET:HE1	1.89	0.54
1:C:92:GLU:HG2	2:C:301:NAD:C2D	2.37	0.54
1:I:117:ASN:HD21	2:I:301:NAD:C6N	2.19	0.54
1:D:218:MET:HA	1:D:218:MET:HE3	1.89	0.54
1:E:113:ILE:HG12	1:E:163:THR:HG23	1.89	0.54
1:E:189:VAL:HA	1:F:218:MET:CE	2.37	0.54
1:H:115:ALA:HB1	1:H:139:MET:HE3	1.87	0.54
1:H:186:GLY:O	1:H:187:PHE:C	2.46	0.54
1:I:164:HIS:HE1	1:I:180:THR:OG1	1.89	0.54
1:C:143:ASN:CA	3:C:404:HOH:O	2.56	0.54
1:E:117:ASN:HA	1:E:139:MET:O	2.08	0.54
1:C:60:THR:HG23	1:C:63:ASP:H	1.73	0.54
1:F:150:LEU:HD11	1:F:179:ILE:CG2	2.38	0.54
1:E:206:GLU:OE1	1:F:191:ARG:NH2	2.40	0.53
1:C:244:MET:HE2	1:C:244:MET:HA	1.91	0.53
1:E:16:ASN:C	1:E:16:ASN:ND2	2.62	0.53
1:F:9:VAL:HG21	1:F:104:ILE:HD11	1.89	0.53
1:B:8:ILE:O	1:B:8:ILE:HG22	2.08	0.53
1:C:273:ARG:O	1:C:275:THR:N	2.42	0.53
1:E:137:ILE:HG21	1:E:167:VAL:HG21	1.91	0.53
1:B:194:CYS:HB3	1:B:244:MET:CE	2.38	0.52
1:I:92:GLU:HG2	2:I:301:NAD:H2D	1.90	0.52
1:D:283:SER:O	1:D:284:LYS:HB2	2.09	0.52
1:B:199:GLU:OE2	1:C:191:ARG:NH1	2.42	0.52
1:F:140:HIS:HB3	1:F:152:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MET:CE	1:A:263:ARG:HE	2.22	0.52
1:G:194:CYS:HB3	1:G:244:MET:CE	2.40	0.52
1:F:244:MET:HA	1:F:244:MET:CE	2.40	0.52
1:I:92:GLU:CG	2:I:301:NAD:H2D	2.40	0.52
1:B:139:MET:HG2	1:B:141:PHE:CE1	2.44	0.52
1:E:38:ALA:HA	1:E:41:LYS:HG2	1.91	0.51
1:E:75:THR:CG2	3:E:405:HOH:O	2.59	0.51
1:I:269:GLY:C	1:I:271:LEU:HD13	2.31	0.51
1:D:167:VAL:O	1:D:171:SER:OG	2.28	0.51
1:G:164:HIS:HE1	1:G:180:THR:OG1	1.92	0.51
1:D:25:VAL:O	1:D:25:VAL:HG12	2.10	0.51
1:F:126:LEU:O	1:F:129:VAL:HG22	2.11	0.51
1:G:120:SER:HA	3:G:407:HOH:O	2.11	0.51
1:C:143:ASN:CB	3:C:404:HOH:O	2.59	0.51
1:I:16:ASN:HB3	1:I:31:MET:HE1	1.93	0.51
1:E:189:VAL:HA	1:F:218:MET:HE2	1.92	0.50
1:G:143:ASN:ND2	2:G:301:NAD:O7N	2.43	0.50
1:I:176:LYS:HE2	3:I:404:HOH:O	2.10	0.50
1:G:194:CYS:C	1:G:244:MET:CE	2.80	0.50
1:H:32:VAL:HG12	1:H:33:ASP:N	2.25	0.50
1:D:216:GLU:OE1	1:G:177:TYR:CD1	2.65	0.50
1:E:88:GLU:OE2	1:E:90:ALA:N	2.42	0.50
1:B:189:VAL:HA	1:C:218:MET:CE	2.42	0.50
1:G:194:CYS:HB3	1:G:244:MET:HE1	1.93	0.50
1:G:283:SER:O	1:G:284:LYS:CB	2.60	0.50
1:D:164:HIS:CE1	1:D:180:THR:OG1	2.65	0.50
1:C:115:ALA:HA	1:C:137:ILE:O	2.11	0.50
1:B:192:ILE:HB	1:C:218:MET:HE1	1.94	0.50
1:E:33:ASP:OD1	1:E:34:ILE:N	2.43	0.49
1:F:269:GLY:C	1:F:271:LEU:HD13	2.32	0.49
1:H:88:GLU:OE2	1:H:90:ALA:N	2.43	0.49
1:I:77:TYR:CD2	1:I:103:GLN:HG2	2.47	0.49
1:I:140:HIS:HB3	1:I:152:GLU:HB3	1.94	0.49
1:H:117:ASN:HA	1:H:139:MET:O	2.13	0.49
1:D:223:ASN:HB3	1:G:225:PRO:HG3	1.95	0.49
1:E:218:MET:CE	1:F:189:VAL:HA	2.42	0.49
1:I:60:THR:HG22	1:I:63:ASP:OD2	2.12	0.49
1:F:92:GLU:HG2	2:F:301:NAD:H2D	1.94	0.49
1:E:32:VAL:HG12	1:E:33:ASP:N	2.28	0.49
1:H:117:ASN:OD1	2:H:301:NAD:H1D	2.13	0.49
1:H:189:VAL:HA	1:I:218:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:MET:HE3	1:I:143:ASN:HB3	1.94	0.48
1:F:164:HIS:HE1	1:F:180:THR:OG1	1.96	0.48
1:G:117:ASN:HA	1:G:139:MET:O	2.14	0.48
1:E:73:GLY:CA	3:E:408:HOH:O	2.60	0.48
1:G:283:SER:O	1:G:284:LYS:HB2	2.14	0.48
1:E:283:SER:HA	1:E:284:LYS:HB3	1.95	0.48
1:F:53:LEU:CB	1:F:59:LEU:HD12	2.43	0.48
1:G:59:LEU:HA	1:G:60:THR:HG23	1.95	0.48
1:E:212:GLU:O	1:E:216:GLU:HG2	2.14	0.48
1:C:277:ARG:NH1	1:C:281:VAL:HG22	2.28	0.48
1:B:85:ILE:HG13	1:B:113:ILE:O	2.14	0.48
1:E:117:ASN:OD1	2:E:301:NAD:H1D	2.13	0.48
1:A:51:ASP:HA	1:A:54:ILE:HD12	1.95	0.48
1:A:59:LEU:HA	1:A:60:THR:HG23	1.95	0.48
1:D:16:ASN:HB3	1:D:46:VAL:HG23	1.96	0.48
1:H:126:LEU:O	1:H:129:VAL:HG22	2.14	0.47
1:A:7:GLY:N	1:A:85:ILE:O	2.43	0.47
1:E:226:ILE:HG13	1:E:227:GLY:N	2.29	0.47
1:E:164:HIS:HE1	1:E:180:THR:OG1	1.96	0.47
1:I:115:ALA:HA	1:I:137:ILE:O	2.14	0.47
1:D:260:MET:CE	1:D:263:ARG:HE	2.27	0.47
1:C:11:ALA:HA	1:C:31:MET:CE	2.45	0.47
1:B:191:ARG:NH1	1:B:256:TYR:OH	2.47	0.47
1:D:12:GLY:HA3	2:D:301:NAD:O5B	2.15	0.47
1:D:59:LEU:CB	1:D:60:THR:HG23	2.44	0.47
1:C:60:THR:HG22	1:C:63:ASP:CG	2.35	0.47
1:I:176:LYS:CE	3:I:404:HOH:O	2.63	0.47
1:C:194:CYS:HA	1:C:240:MET:HE1	1.97	0.47
1:C:150:LEU:HD11	1:C:179:ILE:HG21	1.96	0.47
1:D:218:MET:HE3	1:D:222:CYS:SG	2.55	0.46
1:C:248:TYR:O	1:C:252:ALA:N	2.48	0.46
1:C:60:THR:HG22	1:C:63:ASP:OD2	2.14	0.46
1:F:150:LEU:HD11	1:F:179:ILE:HG21	1.98	0.46
1:G:117:ASN:OD1	2:G:301:NAD:H1D	2.15	0.46
1:H:8:ILE:O	1:H:8:ILE:CG2	2.60	0.46
1:D:260:MET:HE1	1:D:263:ARG:HE	1.80	0.46
1:F:16:ASN:HA	1:F:31:MET:CE	2.44	0.46
1:B:105:ASP:OD1	1:B:131:SER:OG	2.29	0.46
1:I:152:GLU:OE2	1:I:188:VAL:HB	2.16	0.46
1:D:260:MET:HE1	3:D:403:HOH:O	2.11	0.46
1:H:4:ARG:O	1:H:27:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ALA:HA	1:F:137:ILE:O	2.15	0.46
1:A:117:ASN:HA	1:A:139:MET:O	2.16	0.46
1:H:283:SER:HA	1:H:284:LYS:C	2.36	0.46
1:A:219:LYS:O	1:A:223:ASN:HA	2.16	0.46
1:G:92:GLU:HG2	2:G:301:NAD:C2D	2.46	0.46
1:H:226:ILE:HG13	1:H:227:GLY:N	2.30	0.46
1:B:189:VAL:HA	1:C:218:MET:HE2	1.97	0.45
1:G:194:CYS:CB	1:G:244:MET:HE1	2.46	0.45
1:H:20:GLN:O	1:H:24:VAL:HG23	2.16	0.45
1:D:92:GLU:HG2	2:D:301:NAD:C2D	2.46	0.45
1:E:225:PRO:HG3	1:F:223:ASN:HB3	1.98	0.45
1:H:189:VAL:HA	1:I:218:MET:HE2	1.97	0.45
1:C:246:VAL:O	1:C:250:GLU:HB2	2.17	0.45
1:H:218:MET:CE	1:I:189:VAL:HA	2.46	0.45
1:D:92:GLU:HG2	2:D:301:NAD:H2D	1.98	0.45
1:C:145:VAL:O	1:C:176:LYS:NZ	2.49	0.45
1:F:152:GLU:OE2	1:F:188:VAL:HB	2.16	0.45
1:D:127:ALA:HB2	1:D:136:PHE:CD1	2.50	0.45
1:C:140:HIS:HB3	1:C:152:GLU:HB3	1.99	0.45
1:B:244:MET:HE2	1:B:247:LEU:HD12	1.99	0.45
1:D:117:ASN:OD1	2:D:301:NAD:H6N	2.17	0.45
1:G:4:ARG:N	1:G:84:ASP:OD2	2.48	0.45
1:B:16:ASN:C	1:B:16:ASN:HD22	2.19	0.45
1:D:27:LEU:HD21	1:D:173:GLN:NE2	2.32	0.45
1:H:37:ALA:C	3:H:409:HOH:O	2.54	0.44
1:C:16:ASN:HB3	1:C:31:MET:HE1	1.97	0.44
1:G:270:TYR:CD1	1:G:277:ARG:HD3	2.51	0.44
1:H:49:SER:O	1:H:52:ARG:N	2.51	0.44
1:D:281:VAL:CG1	1:E:58:LYS:HD2	2.48	0.44
1:I:105:ASP:OD2	1:I:131:SER:N	2.42	0.44
1:H:216:GLU:O	1:H:217:GLY:C	2.56	0.44
1:C:172:LYS:O	1:C:173:GLN:C	2.53	0.44
1:H:219:LYS:O	1:H:223:ASN:HA	2.18	0.44
1:E:194:CYS:CB	1:E:244:MET:HE1	2.45	0.44
1:A:260:MET:HE1	1:A:263:ARG:HE	1.83	0.44
1:D:186:GLY:O	1:D:187:PHE:C	2.55	0.44
1:G:219:LYS:O	1:G:223:ASN:HA	2.16	0.44
1:H:108:VAL:HG11	1:H:112:VAL:CG1	2.45	0.44
1:B:75:THR:CG2	3:B:408:HOH:O	2.66	0.44
1:C:152:GLU:OE2	1:C:188:VAL:HB	2.17	0.44
1:F:103:GLN:HB2	1:F:103:GLN:HE21	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ASN:OD1	2:G:301:NAD:H6N	2.18	0.44
1:D:140:HIS:HB3	1:D:152:GLU:HB2	2.00	0.44
1:H:212:GLU:O	1:H:216:GLU:HG2	2.18	0.44
1:A:16:ASN:O	1:A:17:GLY:C	2.55	0.44
1:H:91:THR:O	1:H:97:LYS:HD2	2.18	0.44
1:C:164:HIS:CE1	1:C:180:THR:OG1	2.69	0.44
1:B:218:MET:HE2	1:C:189:VAL:HA	2.00	0.44
1:B:137:ILE:HG21	1:B:167:VAL:HG21	1.99	0.43
1:G:117:ASN:ND2	1:G:141:PHE:H	2.11	0.43
1:A:102:LYS:HE3	1:A:129:VAL:HB	2.00	0.43
1:H:92:GLU:HG2	2:H:301:NAD:C2D	2.48	0.43
1:A:140:HIS:HD2	1:A:152:GLU:OE1	2.00	0.43
1:C:259:ALA:HB1	3:C:411:HOH:O	2.18	0.43
1:F:153:LEU:HD22	1:F:167:VAL:HG12	2.01	0.43
1:B:206:GLU:OE1	1:C:191:ARG:NH2	2.52	0.43
1:D:85:ILE:HG13	1:D:113:ILE:O	2.18	0.43
1:H:96:LEU:O	1:H:99:LYS:N	2.52	0.43
1:H:13:THR:N	2:H:301:NAD:O2A	2.50	0.43
1:D:140:HIS:CE1	2:D:301:NAD:H5N	2.54	0.43
1:F:11:ALA:HA	1:F:31:MET:CE	2.49	0.43
1:I:153:LEU:HD22	1:I:167:VAL:HG12	2.00	0.43
1:E:181:VAL:HG12	1:E:182:LYS:O	2.18	0.43
1:G:198:ASN:HD22	1:G:262:MET:CE	2.32	0.43
1:H:115:ALA:CB	1:H:139:MET:HE3	2.49	0.43
1:H:140:HIS:HB3	1:H:152:GLU:HB2	2.00	0.43
1:A:103:GLN:NE2	3:A:410:HOH:O	2.51	0.42
1:C:9:VAL:HG21	1:C:104:ILE:HD11	2.01	0.42
1:D:63:ASP:O	1:D:64:LYS:C	2.56	0.42
1:H:77:TYR:OH	2:H:301:NAD:N1A	2.53	0.42
1:F:60:THR:HG22	1:F:63:ASP:CG	2.38	0.42
1:F:139:MET:CE	1:F:167:VAL:HG13	2.49	0.42
1:I:32:VAL:HA	1:I:74:SER:O	2.19	0.42
1:E:157:LEU:HA	1:E:157:LEU:HD23	1.91	0.42
1:H:16:ASN:C	1:H:16:ASN:HD22	2.23	0.42
1:H:12:GLY:O	1:H:13:THR:C	2.58	0.42
1:H:41:LYS:HD3	3:H:409:HOH:O	2.18	0.42
1:D:17:GLY:HA3	1:D:145:VAL:HB	2.02	0.42
1:E:65:ALA:O	1:E:69:ALA:N	2.47	0.42
1:D:80:LEU:O	1:D:83:THR:OG1	2.36	0.42
1:D:218:MET:HE1	1:D:222:CYS:SG	2.59	0.42
1:B:218:MET:HE1	1:C:189:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:HIS:HE1	1:B:180:THR:OG1	2.02	0.42
1:I:260:MET:CE	3:I:405:HOH:O	2.68	0.42
1:B:191:ARG:O	1:B:191:ARG:HG3	2.19	0.42
1:G:194:CYS:C	1:G:244:MET:HE1	2.40	0.42
1:C:150:LEU:HD11	1:C:179:ILE:CG2	2.49	0.42
1:A:173:GLN:O	1:A:175:GLY:N	2.53	0.42
1:H:34:ILE:CG2	3:H:408:HOH:O	2.60	0.42
1:B:244:MET:CE	1:B:247:LEU:HD12	2.49	0.42
1:H:187:PHE:O	1:H:191:ARG:HB3	2.19	0.42
1:B:192:ILE:HD12	1:C:218:MET:CE	2.48	0.42
1:H:19:ALA:HB1	1:H:29:VAL:HG11	2.02	0.42
1:B:212:GLU:O	1:B:216:GLU:HG2	2.20	0.42
1:H:91:THR:HA	2:H:301:NAD:O3D	2.19	0.41
1:D:145:VAL:O	1:D:176:LYS:NZ	2.41	0.41
1:E:113:ILE:HD11	3:E:410:HOH:O	2.20	0.41
1:H:39:VAL:CG2	1:H:74:SER:O	2.65	0.41
1:C:12:GLY:O	1:C:13:THR:C	2.58	0.41
1:A:92:GLU:N	2:A:301:NAD:O3D	2.53	0.41
1:A:190:ASN:HD22	1:A:190:ASN:HA	1.65	0.41
1:H:119:SER:HA	1:H:140:HIS:CE1	2.55	0.41
1:C:181:VAL:HG12	1:C:182:LYS:O	2.20	0.41
1:D:77:TYR:OH	2:D:301:NAD:N1A	2.53	0.41
1:H:218:MET:HE1	1:I:189:VAL:HA	2.01	0.41
1:E:93:ASN:O	1:E:97:LYS:HB2	2.20	0.41
1:C:244:MET:HA	1:C:244:MET:CE	2.51	0.41
1:A:260:MET:HE2	1:A:263:ARG:HE	1.86	0.41
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.88	0.41
1:D:192:ILE:HG22	1:G:199:GLU:CG	2.51	0.41
1:F:32:VAL:HA	1:F:74:SER:O	2.21	0.41
1:A:241:LEU:HD23	1:A:266:VAL:HG11	2.02	0.41
1:I:10:GLY:O	1:I:15:GLY:HA3	2.21	0.41
1:I:179:ILE:HG21	1:I:179:ILE:HD13	1.73	0.41
1:B:115:ALA:HB1	1:B:139:MET:HE3	2.02	0.41
1:I:103:GLN:HE21	1:I:103:GLN:HB2	1.67	0.41
1:F:59:LEU:HD22	1:F:63:ASP:CB	2.51	0.41
1:E:179:ILE:HD13	1:E:179:ILE:HA	1.91	0.41
1:I:126:LEU:O	1:I:129:VAL:HG22	2.21	0.41
1:C:219:LYS:O	1:C:223:ASN:HA	2.21	0.41
1:A:198:ASN:ND2	1:A:259:ALA:H	2.11	0.41
1:G:145:VAL:HG12	1:G:145:VAL:O	2.21	0.41
1:A:3:ILE:O	1:A:3:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:MET:CE	1:G:263:ARG:HE	2.33	0.41
1:G:126:LEU:O	1:G:129:VAL:HG22	2.21	0.41
1:E:191:ARG:HH11	1:E:191:ARG:CG	2.34	0.40
1:B:244:MET:HA	1:B:244:MET:HE2	2.03	0.40
1:B:167:VAL:O	1:B:171:SER:OG	2.36	0.40
1:A:28:ASN:ND2	1:A:70:ARG:HG3	2.36	0.40
1:D:150:LEU:O	1:D:150:LEU:HD13	2.21	0.40
1:C:117:ASN:ND2	2:C:301:NAD:H1D	2.36	0.40
1:F:11:ALA:HA	1:F:31:MET:HE2	2.03	0.40
1:F:117:ASN:ND2	2:F:301:NAD:H1D	2.37	0.40
1:G:164:HIS:CE1	1:G:180:THR:OG1	2.73	0.40
1:F:283:SER:O	1:F:284:LYS:HB2	2.20	0.40
1:D:74:SER:OG	1:D:75:THR:N	2.55	0.40
1:A:184:SER:O	1:A:185:PRO:C	2.60	0.40
1:A:150:LEU:O	1:A:150:LEU:HD13	2.21	0.40
1:A:93:ASN:O	1:A:97:LYS:HB2	2.21	0.40
1:F:12:GLY:O	1:F:13:THR:C	2.59	0.40
1:A:137:ILE:HG21	1:A:167:VAL:HG21	2.03	0.40
1:I:117:ASN:HD21	2:I:301:NAD:H1D	1.84	0.40
1:G:194:CYS:C	1:G:244:MET:HE3	2.40	0.40
1:E:91:THR:HA	2:E:301:NAD:O3D	2.22	0.40
1:G:59:LEU:HB3	1:G:60:THR:HG23	2.04	0.40
1:D:74:SER:CB	1:D:79:ASP:OD2	2.70	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	281/284 (99%)	257 (92%)	22 (8%)	2 (1%)	26	49
1	B	281/284 (99%)	249 (89%)	29 (10%)	3 (1%)	17	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	281/284 (99%)	264 (94%)	15 (5%)	2 (1%)	26	49
1	D	281/284 (99%)	256 (91%)	24 (8%)	1 (0%)	39	63
1	E	281/284 (99%)	259 (92%)	22 (8%)	0	100	100
1	F	281/284 (99%)	272 (97%)	7 (2%)	2 (1%)	26	49
1	G	281/284 (99%)	259 (92%)	21 (8%)	1 (0%)	39	63
1	H	281/284 (99%)	253 (90%)	28 (10%)	0	100	100
1	I	281/284 (99%)	264 (94%)	15 (5%)	2 (1%)	26	49
All	All	2529/2556 (99%)	2333 (92%)	183 (7%)	13 (0%)	34	58

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	274	LYS
1	C	120	SER
1	F	274	LYS
1	I	274	LYS
1	A	174	LEU
1	B	80	LEU
1	F	120	SER
1	A	144	PRO
1	B	81	LYS
1	B	73	GLY
1	D	144	PRO
1	I	120	SER
1	G	144	PRO

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	227/228 (100%)	205 (90%)	22 (10%)	10	18
1	B	227/228 (100%)	208 (92%)	19 (8%)	14	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	227/228 (100%)	220 (97%)	7 (3%)	47 75
1	D	227/228 (100%)	214 (94%)	13 (6%)	25 48
1	E	227/228 (100%)	215 (95%)	12 (5%)	28 52
1	F	227/228 (100%)	218 (96%)	9 (4%)	38 66
1	G	227/228 (100%)	212 (93%)	15 (7%)	21 39
1	H	227/228 (100%)	212 (93%)	15 (7%)	21 39
1	I	227/228 (100%)	220 (97%)	7 (3%)	47 75
All	All	2043/2052 (100%)	1924 (94%)	119 (6%)	25 47

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	25	VAL
1	A	36	ASP
1	A	40	GLN
1	A	45	THR
1	A	60	THR
1	A	70	ARG
1	A	72	LYS
1	A	75	THR
1	A	79	ASP
1	A	111	ASN
1	A	116	SER
1	A	119	SER
1	A	135	ARG
1	A	150	LEU
1	A	171	SER
1	A	173	GLN
1	A	191	ARG
1	A	192	ILE
1	A	223	ASN
1	A	271	LEU
1	A	283	SER
1	B	4	ARG
1	B	5	THR
1	B	16	ASN
1	B	36	ASP
1	B	40	GLN
1	B	45	THR

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Mol	Chain	Res	Type
1	B	48	SER
1	B	49	SER
1	B	52	ARG
1	B	53	LEU
1	B	111	ASN
1	B	125	LYS
1	B	139	MET
1	B	145	VAL
1	B	153	LEU
1	B	161	ASP
1	B	174	LEU
1	B	191	ARG
1	B	220	LEU
1	C	4	ARG
1	C	66	SER
1	C	76	SER
1	C	179	ILE
1	C	191	ARG
1	C	224	HIS
1	C	271	LEU
1	D	31	MET
1	D	45	THR
1	D	50	LEU
1	D	61	GLU
1	D	70	ARG
1	D	75	THR
1	D	135	ARG
1	D	150	LEU
1	D	171	SER
1	D	191	ARG
1	D	192	ILE
1	D	223	ASN
1	D	271	LEU
1	E	16	ASN
1	E	40	GLN
1	E	56	LYS
1	E	110	GLU
1	E	119	SER
1	E	125	LYS
1	E	145	VAL
1	E	153	LEU
1	E	191	ARG

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Mol	Chain	Res	Type
1	E	220	LEU
1	E	224	HIS
1	E	226	ILE
1	F	60	THR
1	F	66	SER
1	F	96	LEU
1	F	125	LYS
1	F	179	ILE
1	F	191	ARG
1	F	224	HIS
1	F	271	LEU
1	F	274	LYS
1	G	16	ASN
1	G	31	MET
1	G	36	ASP
1	G	45	THR
1	G	49	SER
1	G	60	THR
1	G	70	ARG
1	G	111	ASN
1	G	150	LEU
1	G	162	THR
1	G	177	TYR
1	G	191	ARG
1	G	192	ILE
1	G	223	ASN
1	G	271	LEU
1	H	16	ASN
1	H	41	LYS
1	H	49	SER
1	H	55	LYS
1	H	58	LYS
1	H	110	GLU
1	H	139	MET
1	H	145	VAL
1	H	153	LEU
1	H	161	ASP
1	H	163	THR
1	H	174	LEU
1	H	191	ARG
1	H	220	LEU
1	H	226	ILE

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Mol	Chain	Res	Type
1	I	4	ARG
1	I	48	SER
1	I	191	ARG
1	I	224	HIS
1	I	239	THR
1	I	271	LEU
1	I	284	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	117	ASN
1	A	140	HIS
1	A	164	HIS
1	A	190	ASN
1	A	198	ASN
1	B	16	ASN
1	B	164	HIS
1	B	173	GLN
1	B	190	ASN
1	C	40	GLN
1	C	103	GLN
1	C	117	ASN
1	C	164	HIS
1	D	16	ASN
1	D	28	ASN
1	D	140	HIS
1	D	164	HIS
1	D	190	ASN
1	D	198	ASN
1	D	223	ASN
1	E	16	ASN
1	E	164	HIS
1	E	190	ASN
1	F	40	GLN
1	F	103	GLN
1	F	164	HIS
1	G	28	ASN
1	G	140	HIS
1	G	164	HIS
1	G	190	ASN

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Mol	Chain	Res	Type
1	G	198	ASN
1	G	223	ASN
1	H	16	ASN
1	H	111	ASN
1	H	164	HIS
1	H	173	GLN
1	H	190	ASN
1	H	223	ASN
1	I	40	GLN
1	I	103	GLN
1	I	117	ASN
1	I	164	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

9 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	301	-	38,48,48	1.10	4 (10%)	47,73,73	1.99	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	B	301	-	38,48,48	1.12	4 (10%)	47,73,73	1.92	9 (19%)
2	NAD	C	301	-	38,48,48	1.25	4 (10%)	47,73,73	2.19	8 (17%)
2	NAD	D	301	-	38,48,48	0.98	3 (7%)	47,73,73	1.97	7 (14%)
2	NAD	E	301	-	38,48,48	1.11	4 (10%)	47,73,73	1.94	8 (17%)
2	NAD	F	301	-	38,48,48	1.14	4 (10%)	47,73,73	2.28	10 (21%)
2	NAD	G	301	-	38,48,48	0.99	3 (7%)	47,73,73	2.14	7 (14%)
2	NAD	H	301	-	38,48,48	1.08	4 (10%)	47,73,73	1.96	8 (17%)
2	NAD	I	301	-	38,48,48	1.16	4 (10%)	47,73,73	2.22	7 (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	301	-	-	0/22/62/62	0/5/5/5
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
2	NAD	C	301	-	-	0/22/62/62	0/5/5/5
2	NAD	D	301	-	-	0/22/62/62	0/5/5/5
2	NAD	E	301	-	-	0/22/62/62	0/5/5/5
2	NAD	F	301	-	-	0/22/62/62	0/5/5/5
2	NAD	G	301	-	-	0/22/62/62	0/5/5/5
2	NAD	H	301	-	-	0/22/62/62	0/5/5/5
2	NAD	I	301	-	-	0/22/62/62	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAD	O4B-C1B	2.03	1.43	1.41
2	H	301	NAD	C2A-N3A	2.12	1.36	1.32
2	I	301	NAD	C2A-N3A	2.19	1.36	1.32
2	D	301	NAD	O4B-C1B	2.31	1.44	1.41
2	B	301	NAD	O4B-C1B	2.34	1.44	1.41
2	A	301	NAD	C2A-N3A	2.39	1.36	1.32
2	E	301	NAD	C2A-N3A	2.46	1.36	1.32
2	F	301	NAD	C2A-N3A	2.48	1.36	1.32
2	E	301	NAD	O4B-C1B	2.48	1.44	1.41
2	B	301	NAD	C2A-N3A	2.48	1.36	1.32
2	C	301	NAD	C2A-N3A	2.62	1.36	1.32
2	H	301	NAD	O4B-C1B	2.63	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	NAD	O4B-C1B	2.65	1.44	1.41
2	G	301	NAD	O4D-C1D	2.69	1.44	1.41
2	A	301	NAD	O4B-C1B	2.74	1.44	1.41
2	A	301	NAD	O4D-C1D	2.76	1.44	1.41
2	C	301	NAD	O4B-C1B	2.85	1.44	1.41
2	D	301	NAD	O4D-C1D	2.89	1.44	1.41
2	D	301	NAD	C5A-C4A	2.91	1.47	1.40
2	I	301	NAD	O4B-C1B	2.94	1.44	1.41
2	G	301	NAD	C5A-C4A	3.02	1.47	1.40
2	H	301	NAD	O4D-C1D	3.02	1.45	1.41
2	A	301	NAD	C5A-C4A	3.19	1.47	1.40
2	B	301	NAD	O4D-C1D	3.23	1.45	1.41
2	E	301	NAD	O4D-C1D	3.27	1.45	1.41
2	H	301	NAD	C5A-C4A	3.31	1.48	1.40
2	F	301	NAD	O4D-C1D	3.37	1.45	1.41
2	I	301	NAD	O4D-C1D	3.39	1.45	1.41
2	E	301	NAD	C5A-C4A	3.39	1.48	1.40
2	B	301	NAD	C5A-C4A	3.45	1.48	1.40
2	I	301	NAD	C5A-C4A	3.67	1.48	1.40
2	F	301	NAD	C5A-C4A	3.68	1.48	1.40
2	C	301	NAD	O4D-C1D	3.72	1.45	1.41
2	C	301	NAD	C5A-C4A	3.77	1.49	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	NAD	N3A-C2A-N1A	-9.29	121.78	128.89
2	I	301	NAD	N3A-C2A-N1A	-8.89	122.09	128.89
2	C	301	NAD	N3A-C2A-N1A	-8.69	122.24	128.89
2	D	301	NAD	N3A-C2A-N1A	-8.61	122.30	128.89
2	F	301	NAD	N3A-C2A-N1A	-8.31	122.53	128.89
2	A	301	NAD	N3A-C2A-N1A	-7.90	122.85	128.89
2	H	301	NAD	N3A-C2A-N1A	-7.14	123.43	128.89
2	E	301	NAD	N3A-C2A-N1A	-6.60	123.84	128.89
2	B	301	NAD	N3A-C2A-N1A	-6.48	123.93	128.89
2	B	301	NAD	C4A-C5A-N7A	-4.87	105.00	109.48
2	E	301	NAD	C4A-C5A-N7A	-4.55	105.30	109.48
2	H	301	NAD	C4A-C5A-N7A	-4.53	105.31	109.48
2	D	301	NAD	C4A-C5A-N7A	-4.06	105.74	109.48
2	G	301	NAD	C1B-N9A-C4A	-3.83	121.16	126.94
2	I	301	NAD	C4A-C5A-N7A	-3.61	106.16	109.48
2	A	301	NAD	C4A-C5A-N7A	-3.56	106.20	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	NAD	C4A-C5A-N7A	-3.42	106.33	109.48
2	F	301	NAD	PN-O3-PA	-3.08	124.07	132.73
2	D	301	NAD	C1B-N9A-C4A	-2.98	122.44	126.94
2	C	301	NAD	C4A-C5A-N7A	-2.98	106.74	109.48
2	G	301	NAD	C2B-C1B-N9A	-2.75	110.09	114.29
2	A	301	NAD	C1B-N9A-C4A	-2.73	122.81	126.94
2	B	301	NAD	O7N-C7N-C3N	-2.72	116.62	119.59
2	H	301	NAD	PN-O3-PA	-2.61	125.41	132.73
2	E	301	NAD	PN-O3-PA	-2.60	125.43	132.73
2	F	301	NAD	C2B-C1B-N9A	-2.58	110.34	114.29
2	H	301	NAD	C1B-N9A-C4A	-2.58	123.04	126.94
2	G	301	NAD	C4B-O4B-C1B	-2.58	106.89	109.72
2	D	301	NAD	C2B-C1B-N9A	-2.58	110.36	114.29
2	F	301	NAD	C4A-C5A-N7A	-2.47	107.21	109.48
2	C	301	NAD	O7N-C7N-N7N	-2.40	119.21	122.59
2	B	301	NAD	PN-O3-PA	-2.40	126.00	132.73
2	F	301	NAD	C4B-O4B-C1B	-2.35	107.14	109.72
2	B	301	NAD	C1B-N9A-C4A	-2.35	123.40	126.94
2	A	301	NAD	C2B-C1B-N9A	-2.21	110.92	114.29
2	E	301	NAD	C1B-N9A-C4A	-2.20	123.62	126.94
2	I	301	NAD	C1B-N9A-C4A	-2.16	123.69	126.94
2	D	301	NAD	C5N-C4N-C3N	-2.06	117.74	120.33
2	C	301	NAD	C2B-C1B-N9A	-2.04	111.18	114.29
2	F	301	NAD	C2D-C3D-C4D	-2.04	98.43	102.61
2	F	301	NAD	C2A-N1A-C6A	2.28	122.84	118.77
2	I	301	NAD	C4D-O4D-C1D	2.33	112.27	109.72
2	F	301	NAD	O4B-C4B-C3B	2.34	109.85	105.15
2	H	301	NAD	C4D-O4D-C1D	2.42	112.38	109.72
2	I	301	NAD	C2A-N1A-C6A	2.42	123.10	118.77
2	C	301	NAD	C4D-O4D-C1D	2.57	112.55	109.72
2	E	301	NAD	C4D-O4D-C1D	2.65	112.63	109.72
2	C	301	NAD	C3N-C7N-N7N	2.76	120.83	117.82
2	E	301	NAD	C3N-C7N-N7N	2.78	120.86	117.82
2	B	301	NAD	C4D-O4D-C1D	2.83	112.83	109.72
2	H	301	NAD	C3N-C7N-N7N	3.08	121.18	117.82
2	H	301	NAD	O4B-C1B-N9A	3.55	115.54	108.10
2	B	301	NAD	O4B-C1B-N9A	3.65	115.75	108.10
2	I	301	NAD	O4B-C1B-N9A	3.66	115.76	108.10
2	E	301	NAD	O4B-C1B-N9A	3.78	116.02	108.10
2	D	301	NAD	O4D-C1D-N1N	3.93	112.45	108.13
2	B	301	NAD	C3N-C7N-N7N	4.43	122.67	117.82
2	A	301	NAD	O4B-C1B-N9A	4.49	117.50	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAD	O4B-C1B-N9A	4.69	117.92	108.10
2	F	301	NAD	O4B-C1B-N9A	4.70	117.94	108.10
2	B	301	NAD	O4D-C1D-N1N	4.79	113.39	108.13
2	G	301	NAD	O4D-C1D-N1N	4.86	113.47	108.13
2	D	301	NAD	O4B-C1B-N9A	4.94	118.44	108.10
2	G	301	NAD	O4B-C1B-N9A	5.39	119.39	108.10
2	H	301	NAD	O4D-C1D-N1N	6.17	114.91	108.13
2	A	301	NAD	O4D-C1D-N1N	6.23	114.97	108.13
2	E	301	NAD	O4D-C1D-N1N	6.66	115.45	108.13
2	C	301	NAD	O4D-C1D-N1N	7.38	116.24	108.13
2	I	301	NAD	O4D-C1D-N1N	8.19	117.13	108.13
2	F	301	NAD	O4D-C1D-N1N	8.30	117.25	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	3	0
2	C	301	NAD	4	0
2	D	301	NAD	6	0
2	E	301	NAD	2	0
2	F	301	NAD	4	0
2	G	301	NAD	5	0
2	H	301	NAD	5	0
2	I	301	NAD	7	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	283/284 (99%)	1.52	80 (28%)	1	0	43, 68, 108, 129	0
1	B	283/284 (99%)	1.66	77 (27%)	1	0	40, 74, 109, 127	0
1	C	283/284 (99%)	0.95	37 (13%)	5	3	42, 56, 73, 112	0
1	D	283/284 (99%)	1.74	98 (34%)	0	0	43, 66, 110, 129	0
1	E	283/284 (99%)	1.82	87 (30%)	1	0	41, 75, 112, 130	0
1	F	283/284 (99%)	1.08	45 (15%)	3	1	42, 55, 73, 122	0
1	G	283/284 (99%)	1.95	104 (36%)	0	0	43, 67, 109, 139	0
1	H	283/284 (99%)	1.81	91 (32%)	1	0	41, 75, 112, 131	0
1	I	283/284 (99%)	1.12	50 (17%)	2	1	42, 55, 72, 102	0
All	All	2547/2556 (99%)	1.52	669 (26%)	1	0	40, 62, 107, 139	0

All (669) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	69	ALA	18.3
1	B	2	SER	16.5
1	E	39	VAL	14.4
1	H	9	VAL	11.8
1	B	283	SER	11.6
1	H	15	GLY	11.5
1	H	30	VAL	11.1
1	D	59	LEU	11.1
1	E	72	LYS	11.0
1	G	82	ALA	10.7
1	H	78	ASP	10.3
1	H	34	ILE	10.1
1	E	32	VAL	9.7
1	G	11	ALA	9.2
1	B	13	THR	9.1

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Mol	Chain	Res	Type	RSRZ
1	H	5	THR	9.1
1	G	27	LEU	8.9
1	E	85	ILE	8.9
1	G	73	GLY	8.7
1	B	3	ILE	8.7
1	G	54	ILE	8.6
1	I	281	VAL	8.5
1	G	40	GLN	8.5
1	E	82	ALA	8.3
1	D	192	ILE	8.2
1	H	76	SER	8.1
1	B	14	MET	7.9
1	E	6	VAL	7.9
1	G	119	SER	7.9
1	A	174	LEU	7.8
1	B	36	ASP	7.8
1	E	79	ASP	7.7
1	H	56	LYS	7.7
1	E	113	ILE	7.6
1	G	57	GLU	7.6
1	G	284	LYS	7.5
1	A	176	LYS	7.5
1	E	66	SER	7.5
1	D	70	ARG	7.5
1	H	86	VAL	7.4
1	G	47	ALA	7.3
1	E	160	SER	7.2
1	B	27	LEU	7.1
1	D	18	ILE	7.0
1	G	113	ILE	6.9
1	D	7	GLY	6.9
1	E	10	GLY	6.9
1	G	62	ALA	6.7
1	D	284	LYS	6.7
1	I	2	SER	6.6
1	G	24	VAL	6.5
1	D	149	ALA	6.5
1	I	123	ILE	6.5
1	D	137	ILE	6.4
1	B	31	MET	6.4
1	B	281	VAL	6.3
1	D	14	MET	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	207	GLY	6.3
1	H	91	THR	6.2
1	H	133	ALA	6.2
1	E	107	ILE	6.1
1	E	101	LEU	6.1
1	A	80	LEU	6.1
1	B	38	ALA	6.0
1	B	77	TYR	6.0
1	E	70	ARG	6.0
1	H	146	PRO	6.0
1	E	177	TYR	5.9
1	H	58	LYS	5.8
1	E	40	GLN	5.8
1	D	4	ARG	5.7
1	G	65	ALA	5.5
1	E	30	VAL	5.5
1	A	27	LEU	5.5
1	E	11	ALA	5.5
1	E	37	ALA	5.5
1	H	170	LEU	5.4
1	G	50	LEU	5.4
1	G	107	ILE	5.4
1	A	53	LEU	5.3
1	E	56	LYS	5.3
1	D	71	ILE	5.2
1	H	32	VAL	5.1
1	G	61	GLU	5.1
1	C	283	SER	5.1
1	E	43	VAL	5.1
1	D	231	LEU	5.1
1	B	110	GLU	5.0
1	B	106	GLY	5.0
1	F	226	ILE	5.0
1	D	58	LYS	5.0
1	A	86	VAL	5.0
1	D	25	VAL	5.0
1	I	9	VAL	5.0
1	E	38	ALA	5.0
1	G	16	ASN	4.9
1	H	41	LYS	4.9
1	I	269	GLY	4.9
1	B	147	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	172	LYS	4.9
1	A	95	ASP	4.9
1	I	265	MET	4.8
1	H	143	ASN	4.8
1	A	73	GLY	4.8
1	H	221	GLY	4.8
1	H	35	SER	4.8
1	B	44	ALA	4.8
1	G	201	PHE	4.8
1	B	101	LEU	4.8
1	G	76	SER	4.7
1	B	45	THR	4.7
1	A	279	VAL	4.7
1	A	71	ILE	4.7
1	I	217	GLY	4.7
1	E	22	CYS	4.7
1	G	23	ALA	4.7
1	I	131	SER	4.6
1	D	85	ILE	4.6
1	E	46	VAL	4.6
1	A	84	ASP	4.6
1	A	38	ALA	4.6
1	B	284	LYS	4.5
1	A	52	ARG	4.5
1	G	281	VAL	4.5
1	D	60	THR	4.5
1	B	67	ALA	4.5
1	E	59	LEU	4.4
1	E	80	LEU	4.4
1	E	7	GLY	4.4
1	A	34	ILE	4.4
1	E	35	SER	4.4
1	A	68	LEU	4.4
1	I	10	GLY	4.4
1	B	11	ALA	4.4
1	H	57	GLU	4.4
1	A	77	TYR	4.4
1	G	103	GLN	4.4
1	G	72	LYS	4.3
1	B	182	LYS	4.3
1	E	4	ARG	4.3
1	G	20	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	150	LEU	4.3
1	H	27	LEU	4.3
1	G	89	ALA	4.3
1	F	271	LEU	4.3
1	H	99	LYS	4.3
1	G	147	VAL	4.3
1	H	112	VAL	4.3
1	B	62	ALA	4.3
1	G	26	GLY	4.3
1	G	36	ASP	4.3
1	E	67	ALA	4.3
1	H	284	LYS	4.2
1	G	115	ALA	4.2
1	B	60	THR	4.2
1	B	43	VAL	4.2
1	C	27	LEU	4.2
1	H	177	TYR	4.2
1	D	162	THR	4.2
1	G	29	VAL	4.2
1	D	8	ILE	4.2
1	H	106	GLY	4.2
1	E	47	ALA	4.2
1	C	167	VAL	4.2
1	F	2	SER	4.1
1	B	121	ILE	4.1
1	D	50	LEU	4.1
1	C	143	ASN	4.1
1	H	48	SER	4.1
1	H	84	ASP	4.1
1	H	88	GLU	4.1
1	G	121	ILE	4.1
1	H	59	LEU	4.1
1	A	83	THR	4.1
1	H	179	ILE	4.1
1	B	26	GLY	4.1
1	D	52	ARG	4.1
1	B	114	ILE	4.1
1	D	28	ASN	4.1
1	H	135	ARG	4.1
1	D	3	ILE	4.0
1	E	145	VAL	4.0
1	B	139	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	90	ALA	4.0
1	G	87	ILE	4.0
1	H	145	VAL	3.9
1	E	176	LYS	3.9
1	C	244	MET	3.9
1	E	50	LEU	3.9
1	E	62	ALA	3.9
1	E	132	ARG	3.9
1	G	146	PRO	3.9
1	B	214	ILE	3.9
1	G	55	LYS	3.9
1	E	94	TYR	3.9
1	D	188	VAL	3.9
1	F	258	PRO	3.9
1	G	216	GLU	3.9
1	H	61	GLU	3.9
1	H	141	PHE	3.9
1	G	104	ILE	3.9
1	H	33	ASP	3.9
1	H	62	ALA	3.9
1	A	275	THR	3.8
1	F	80	LEU	3.8
1	C	218	MET	3.8
1	D	67	ALA	3.8
1	B	91	THR	3.8
1	B	209	ALA	3.8
1	G	96	LEU	3.8
1	B	25	VAL	3.7
1	D	193	LEU	3.7
1	I	73	GLY	3.7
1	G	37	ALA	3.7
1	A	24	VAL	3.7
1	B	95	ASP	3.7
1	E	167	VAL	3.7
1	G	39	VAL	3.7
1	B	126	LEU	3.7
1	D	118	THR	3.7
1	A	232	ALA	3.7
1	A	81	LYS	3.7
1	E	51	ASP	3.7
1	H	19	ALA	3.7
1	D	24	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	35	SER	3.6
1	G	240	MET	3.6
1	H	94	TYR	3.6
1	G	44	ALA	3.6
1	G	194	CYS	3.6
1	H	139	MET	3.6
1	H	101	LEU	3.6
1	G	141	PHE	3.6
1	D	2	SER	3.6
1	B	39	VAL	3.6
1	F	153	LEU	3.6
1	D	72	LYS	3.6
1	F	81	LYS	3.6
1	H	73	GLY	3.6
1	H	77	TYR	3.5
1	G	170	LEU	3.5
1	C	139	MET	3.5
1	H	40	GLN	3.5
1	A	237	LEU	3.5
1	H	29	VAL	3.5
1	G	52	ARG	3.5
1	G	85	ILE	3.5
1	I	51	ASP	3.5
1	G	203	VAL	3.5
1	C	252	ALA	3.5
1	B	34	ILE	3.5
1	C	205	GLY	3.5
1	I	208	LEU	3.5
1	C	52	ARG	3.5
1	E	271	LEU	3.5
1	G	167	VAL	3.5
1	B	41	LYS	3.5
1	B	52	ARG	3.5
1	A	51	ASP	3.5
1	C	87	ILE	3.5
1	E	130	THR	3.5
1	G	100	ILE	3.4
1	D	6	VAL	3.4
1	D	42	GLY	3.4
1	G	164	HIS	3.4
1	E	3	ILE	3.4
1	A	31	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	77	TYR	3.4
1	E	81	LYS	3.4
1	D	80	LEU	3.4
1	G	276	GLY	3.3
1	D	69	ALA	3.3
1	F	71	ILE	3.3
1	A	177	TYR	3.3
1	H	114	ILE	3.3
1	F	172	LYS	3.3
1	H	220	LEU	3.3
1	H	63	ASP	3.3
1	F	30	VAL	3.3
1	D	77	TYR	3.3
1	I	177	TYR	3.3
1	E	110	GLU	3.3
1	E	117	ASN	3.3
1	D	74	SER	3.3
1	D	87	ILE	3.3
1	E	102	LYS	3.3
1	G	33	ASP	3.3
1	H	238	ASP	3.3
1	B	30	VAL	3.3
1	D	126	LEU	3.3
1	F	257	ARG	3.3
1	C	90	ALA	3.3
1	G	79	ASP	3.2
1	B	85	ILE	3.2
1	D	259	ALA	3.2
1	A	55	LYS	3.2
1	F	4	ARG	3.2
1	B	73	GLY	3.2
1	D	57	GLU	3.2
1	H	126	LEU	3.2
1	A	129	VAL	3.2
1	F	187	PHE	3.2
1	G	114	ILE	3.2
1	H	31	MET	3.2
1	H	98	VAL	3.2
1	G	196	MET	3.2
1	H	274	LYS	3.2
1	H	22	CYS	3.1
1	C	228	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	284	LYS	3.1
1	H	75	THR	3.1
1	G	282	TYR	3.1
1	D	111	ASN	3.1
1	D	246	VAL	3.1
1	A	251	PHE	3.1
1	E	9	VAL	3.1
1	F	32	VAL	3.1
1	E	155	ARG	3.1
1	D	81	LYS	3.1
1	E	33	ASP	3.1
1	E	134	ASP	3.1
1	A	3	ILE	3.1
1	A	154	ILE	3.1
1	E	114	ILE	3.1
1	A	11	ALA	3.1
1	E	87	ILE	3.1
1	I	273	ARG	3.1
1	D	54	ILE	3.1
1	H	74	SER	3.1
1	G	8	ILE	3.0
1	A	41	LYS	3.0
1	C	182	LYS	3.0
1	F	274	LYS	3.0
1	D	128	ALA	3.0
1	E	74	SER	3.0
1	G	160	SER	3.0
1	G	6	VAL	3.0
1	G	80	LEU	3.0
1	I	180	THR	3.0
1	D	34	ILE	3.0
1	A	57	GLU	3.0
1	D	174	LEU	3.0
1	C	101	LEU	3.0
1	I	130	THR	3.0
1	B	137	ILE	3.0
1	C	56	LYS	3.0
1	F	151	VAL	3.0
1	B	150	LEU	3.0
1	B	277	ARG	3.0
1	H	18	ILE	3.0
1	I	24	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	277	ARG	3.0
1	E	265	MET	3.0
1	B	154	ILE	3.0
1	D	175	GLY	2.9
1	D	282	TYR	2.9
1	B	17	GLY	2.9
1	B	57	GLU	2.9
1	F	247	LEU	2.9
1	H	166	ALA	2.9
1	D	142	PHE	2.9
1	C	80	LEU	2.9
1	G	94	TYR	2.9
1	H	83	THR	2.9
1	A	116	SER	2.9
1	E	135	ARG	2.9
1	G	117	ASN	2.9
1	C	243	VAL	2.9
1	E	204	LEU	2.9
1	I	35	SER	2.9
1	E	65	ALA	2.9
1	D	27	LEU	2.9
1	A	18	ILE	2.8
1	B	8	ILE	2.8
1	B	29	VAL	2.8
1	E	283	SER	2.8
1	H	82	ALA	2.8
1	E	77	TYR	2.8
1	A	235	ILE	2.8
1	H	36	ASP	2.8
1	I	179	ILE	2.8
1	A	9	VAL	2.8
1	A	181	VAL	2.8
1	F	58	LYS	2.8
1	G	226	ILE	2.8
1	D	127	ALA	2.8
1	B	216	GLU	2.8
1	E	178	PRO	2.8
1	A	240	MET	2.8
1	D	147	VAL	2.8
1	D	62	ALA	2.8
1	F	225	PRO	2.8
1	C	229	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	208	LEU	2.8
1	F	87	ILE	2.8
1	E	83	THR	2.8
1	H	16	ASN	2.8
1	E	76	SER	2.8
1	F	217	GLY	2.8
1	D	110	GLU	2.8
1	A	145	VAL	2.8
1	G	30	VAL	2.8
1	G	149	ALA	2.8
1	E	73	GLY	2.8
1	F	270	TYR	2.7
1	H	228	PRO	2.7
1	C	111	ASN	2.7
1	C	175	GLY	2.7
1	G	77	TYR	2.7
1	B	129	VAL	2.7
1	A	20	GLN	2.7
1	A	252	ALA	2.7
1	A	49	SER	2.7
1	B	96	LEU	2.7
1	B	237	LEU	2.7
1	C	107	ILE	2.7
1	F	281	VAL	2.7
1	B	37	ALA	2.7
1	H	157	LEU	2.7
1	G	140	HIS	2.7
1	B	143	ASN	2.7
1	D	143	ASN	2.7
1	H	12	GLY	2.7
1	B	55	LYS	2.7
1	E	131	SER	2.7
1	B	71	ILE	2.7
1	C	227	GLY	2.7
1	H	107	ILE	2.7
1	D	177	TYR	2.7
1	I	29	VAL	2.7
1	G	242	ALA	2.7
1	I	268	ALA	2.7
1	E	18	ILE	2.6
1	A	44	ALA	2.6
1	D	53	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	2.6
1	G	273	ARG	2.6
1	B	136	PHE	2.6
1	D	38	ALA	2.6
1	A	173	GLN	2.6
1	D	153	LEU	2.6
1	I	101	LEU	2.6
1	I	79	ASP	2.6
1	I	226	ILE	2.6
1	B	47	ALA	2.6
1	G	177	TYR	2.6
1	H	72	LYS	2.6
1	G	179	ILE	2.6
1	A	99	LYS	2.6
1	B	48	SER	2.6
1	C	151	VAL	2.6
1	I	188	VAL	2.6
1	H	115	ALA	2.6
1	G	245	GLU	2.6
1	H	50	LEU	2.6
1	H	80	LEU	2.6
1	A	117	ASN	2.6
1	I	283	SER	2.6
1	A	250	GLU	2.6
1	D	212	GLU	2.6
1	I	225	PRO	2.6
1	B	155	ARG	2.6
1	A	168	GLU	2.6
1	B	86	VAL	2.6
1	D	141	PHE	2.6
1	D	96	LEU	2.5
1	D	121	ILE	2.5
1	H	258	PRO	2.5
1	D	169	ALA	2.5
1	A	247	LEU	2.5
1	E	154	ILE	2.5
1	E	282	TYR	2.5
1	A	6	VAL	2.5
1	I	260	MET	2.5
1	D	19	ALA	2.5
1	D	281	VAL	2.5
1	E	99	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	276	GLY	2.5
1	D	271	LEU	2.5
1	I	86	VAL	2.5
1	H	52	ARG	2.5
1	G	78	ASP	2.5
1	G	230	ALA	2.5
1	I	34	ILE	2.5
1	I	113	ILE	2.5
1	I	187	PHE	2.5
1	F	100	ILE	2.4
1	H	242	ALA	2.4
1	D	250	GLU	2.4
1	G	31	MET	2.4
1	A	143	ASN	2.4
1	I	94	TYR	2.4
1	E	141	PHE	2.4
1	D	30	VAL	2.4
1	C	118	THR	2.4
1	C	55	LYS	2.4
1	F	141	PHE	2.4
1	F	177	TYR	2.4
1	A	8	ILE	2.4
1	A	7	GLY	2.4
1	D	176	LYS	2.4
1	E	284	LYS	2.4
1	H	129	VAL	2.4
1	A	283	SER	2.4
1	E	208	LEU	2.4
1	H	197	ILE	2.4
1	I	18	ILE	2.4
1	A	136	PHE	2.4
1	D	228	PRO	2.4
1	A	30	VAL	2.4
1	D	45	THR	2.4
1	D	239	THR	2.4
1	G	256	TYR	2.4
1	B	74	SER	2.4
1	H	282	TYR	2.3
1	C	120	SER	2.3
1	C	173	GLN	2.3
1	D	225	PRO	2.3
1	E	217	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	26	GLY	2.3
1	F	50	LEU	2.3
1	I	170	LEU	2.3
1	A	72	LYS	2.3
1	G	56	LYS	2.3
1	I	90	ALA	2.3
1	B	9	VAL	2.3
1	B	87	ILE	2.3
1	A	141	PHE	2.3
1	A	21	ALA	2.3
1	D	98	VAL	2.3
1	G	93	ASN	2.3
1	H	235	ILE	2.3
1	I	231	LEU	2.3
1	E	86	VAL	2.3
1	I	104	ILE	2.3
1	I	4	ARG	2.3
1	D	173	GLN	2.3
1	A	202	CYS	2.3
1	G	283	SER	2.3
1	A	32	VAL	2.3
1	F	24	VAL	2.3
1	I	181	VAL	2.3
1	D	135	ARG	2.3
1	B	195	PRO	2.3
1	D	219	LYS	2.3
1	F	122	SER	2.3
1	F	171	SER	2.3
1	A	179	ILE	2.3
1	B	75	THR	2.3
1	F	282	TYR	2.3
1	D	276	GLY	2.3
1	E	42	GLY	2.3
1	G	45	THR	2.3
1	G	123	ILE	2.3
1	C	68	LEU	2.3
1	A	161	ASP	2.3
1	D	283	SER	2.3
1	E	223	ASN	2.3
1	H	44	ALA	2.3
1	E	100	ILE	2.3
1	F	121	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	68	LEU	2.2
1	G	110	GLU	2.2
1	C	232	ALA	2.2
1	E	279	VAL	2.2
1	G	270	TYR	2.2
1	H	87	ILE	2.2
1	B	220	LEU	2.2
1	G	225	PRO	2.2
1	A	26	GLY	2.2
1	H	11	ALA	2.2
1	E	162	THR	2.2
1	A	267	ALA	2.2
1	B	232	ALA	2.2
1	C	217	GLY	2.2
1	H	26	GLY	2.2
1	I	164	HIS	2.2
1	I	151	VAL	2.2
1	H	113	ILE	2.2
1	D	234	MET	2.2
1	E	108	VAL	2.2
1	D	104	ILE	2.2
1	D	273	ARG	2.2
1	F	3	ILE	2.2
1	H	239	THR	2.2
1	I	174	LEU	2.2
1	G	74	SER	2.2
1	C	110	GLU	2.2
1	A	167	VAL	2.2
1	G	266	VAL	2.2
1	A	75	THR	2.2
1	A	241	LEU	2.2
1	D	103	GLN	2.2
1	C	73	GLY	2.2
1	D	183	ASN	2.2
1	D	99	LYS	2.2
1	I	182	LYS	2.2
1	A	22	CYS	2.2
1	G	204	LEU	2.2
1	A	64	LYS	2.2
1	A	70	ARG	2.2
1	H	222	CYS	2.2
1	F	137	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	193	LEU	2.1
1	G	235	ILE	2.1
1	F	276	GLY	2.1
1	B	97	LYS	2.1
1	E	98	VAL	2.1
1	G	173	GLN	2.1
1	C	104	ILE	2.1
1	B	280	TYR	2.1
1	C	126	LEU	2.1
1	D	189	VAL	2.1
1	G	43	VAL	2.1
1	G	108	VAL	2.1
1	F	139	MET	2.1
1	G	3	ILE	2.1
1	E	199	GLU	2.1
1	G	58	LYS	2.1
1	E	78	ASP	2.1
1	D	9	VAL	2.1
1	D	101	LEU	2.1
1	B	125	LYS	2.1
1	D	97	LYS	2.1
1	F	134	ASP	2.1
1	H	105	ASP	2.1
1	D	204	LEU	2.1
1	H	132	ARG	2.1
1	G	163	THR	2.1
1	I	43	VAL	2.1
1	F	284	LYS	2.1
1	C	270	TYR	2.1
1	F	37	ALA	2.1
1	A	206	GLU	2.1
1	I	271	LEU	2.1
1	G	83	THR	2.1
1	B	141	PHE	2.1
1	G	148	MET	2.1
1	A	280	TYR	2.1
1	G	71	ILE	2.1
1	H	192	ILE	2.1
1	G	64	LYS	2.1
1	B	282	TYR	2.1
1	D	22	CYS	2.1
1	D	170	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	147	VAL	2.0
1	G	275	THR	2.0
1	A	114	ILE	2.0
1	G	174	LEU	2.0
1	I	147	VAL	2.0
1	F	154	ILE	2.0
1	I	142	PHE	2.0
1	F	140	HIS	2.0
1	E	2	SER	2.0
1	H	122	SER	2.0
1	F	117	ASN	2.0
1	H	64	LYS	2.0
1	D	5	THR	2.0
1	E	251	PHE	2.0
1	A	100	ILE	2.0
1	I	196	MET	2.0
1	G	219	LYS	2.0
1	A	96	LEU	2.0
1	D	256	TYR	2.0
1	B	112	VAL	2.0
1	D	46	VAL	2.0
1	F	180	THR	2.0
1	I	83	THR	2.0
1	A	144	PRO	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	C	301	44/44	0.63	0.49	3.34	60,82,165,171	0
2	NAD	I	301	44/44	0.60	0.50	2.89	56,91,149,158	0
2	NAD	G	301	44/44	0.61	0.60	1.80	87,126,180,188	0
2	NAD	D	301	44/44	0.66	0.39	1.02	83,121,160,166	0
2	NAD	A	301	44/44	0.53	0.39	0.93	73,117,158,162	0
2	NAD	E	301	44/44	0.57	0.40	0.76	96,130,150,160	0
2	NAD	F	301	44/44	0.77	0.27	0.32	59,85,157,165	0
2	NAD	H	301	44/44	0.50	0.40	0.02	93,129,151,159	0
2	NAD	B	301	44/44	0.68	0.28	-0.43	83,122,146,162	0

6.5 Other polymers (i)

There are no such residues in this entry.