Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:59 AM GMT

PDB ID	:	2VHX
Title	:	CRYSTAL STRUCTURE OF THE TERNARY COMPLEX OF L-ALANINE DEHYDROGENASE FROM MYCOBACTERIUM TUBERCULOSIS WITH NAD+ AND PYRUVATE
Authors	:	Agren, D.; Schneider, G.
Deposited on	:	2007-11-26
Resolution	:	2.00 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:

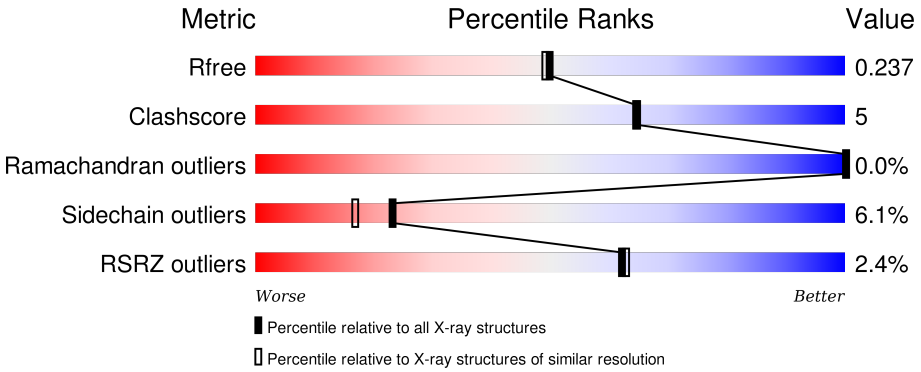
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	377	2% 82% 12%
1	B	377	3% 86% 10%
1	C	377	4% 84% 11%
1	D	377	2% 84% 11%
1	E	377	3% 87% 10%

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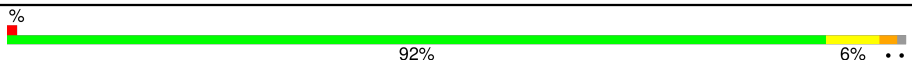
Mol	Chain	Length	Quality of chain
1	F	377	

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
3	PYR	A	1373	-	-	X	-
3	PYR	B	1373	-	-	-	X
3	PYR	C	1371	-	-	-	X
3	PYR	D	1371	-	-	-	X
3	PYR	E	1374	-	-	X	X
3	PYR	F	1375	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17715 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.

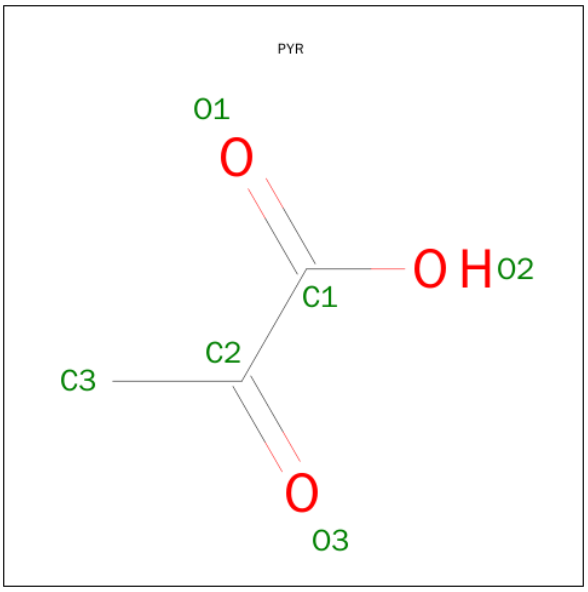
- Molecule 1 is a protein called ALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	4	0
			2727	1716	482	514	15			
1	B	368	Total	C	N	O	S	0	1	0
			2707	1701	477	516	13			
1	C	365	Total	C	N	O	S	0	0	0
			2682	1686	472	511	13			
1	D	367	Total	C	N	O	S	0	3	0
			2712	1706	478	513	15			
1	E	373	Total	C	N	O	S	0	1	0
			2742	1724	485	519	14			
1	F	373	Total	C	N	O	S	0	1	0
			2742	1724	485	519	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

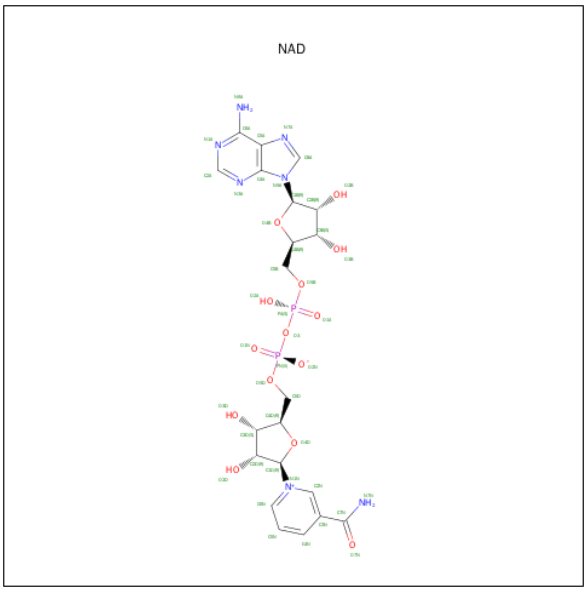
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

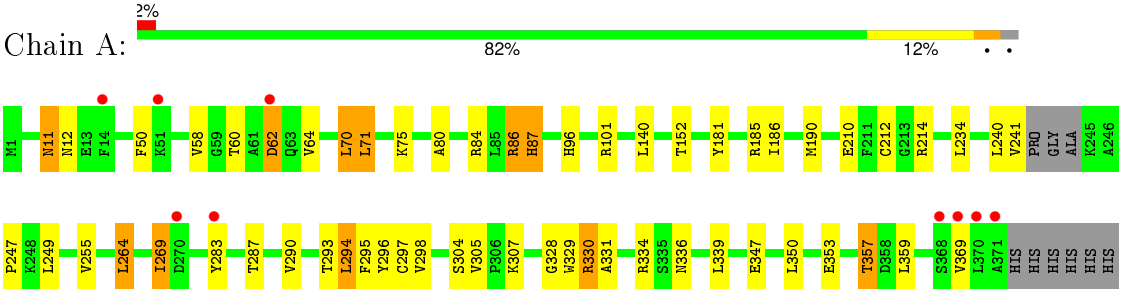
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	184	Total	O	0	0
			184	184		
5	B	228	Total	O	0	0
			228	228		
5	C	185	Total	O	0	0
			185	185		
5	D	232	Total	O	0	0
			232	232		
5	E	195	Total	O	0	0
			195	195		
5	F	252	Total	O	0	0
			252	252		

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.

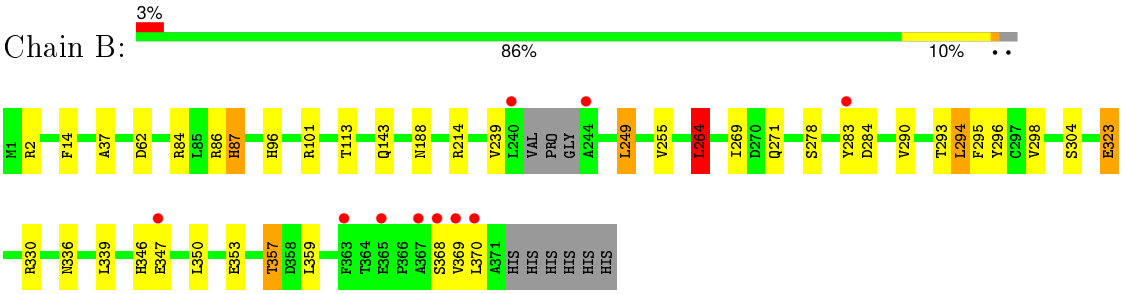
- Molecule 1: ALANINE DEHYDROGENASE

Chain A:



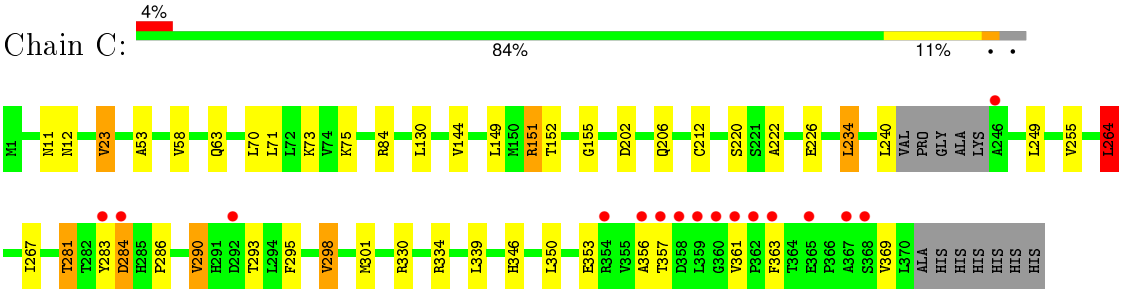
- Molecule 1: ALANINE DEHYDROGENASE

Chain B:



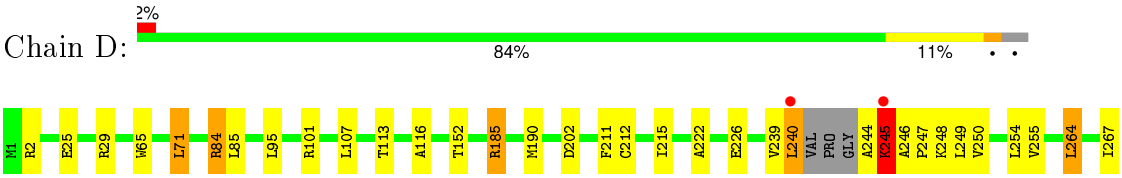
- Molecule 1: ALANINE DEHYDROGENASE

Chain C:



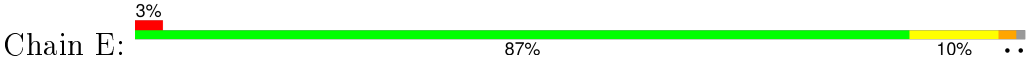
- Molecule 1: ALANINE DEHYDROGENASE

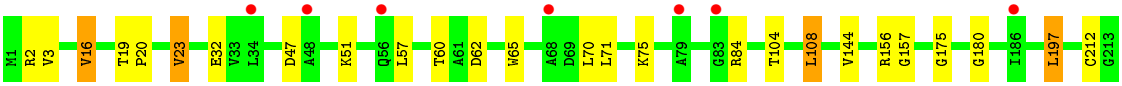
Chain D:



• Molecule 1: ALANINE DEHYDROGENASE

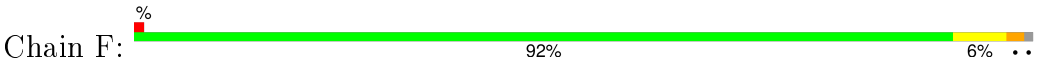
Chain E:

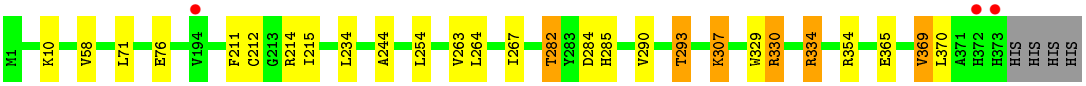




• Molecule 1: ALANINE DEHYDROGENASE

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	176.25Å 171.77Å 98.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 61.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (40.00-2.00) 90.6 (61.29-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.210 0.206 , 0.237	Depositor DCC
R_{free} test set	9182 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.7	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	8 of 182008 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17715	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: MG, PYR, 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	0.71	0/2787	0.82	3/3793 (0.1%)
1	B	0.78	2/2755 (0.1%)	0.81	2/3751 (0.1%)
1	C	0.73	0/2730	0.79	2/3718 (0.1%)
1	D	0.73	0/2769	0.81	7/3769 (0.2%)
1	E	0.62	0/2797	0.76	4/3811 (0.1%)
1	F	0.74	0/2797	0.77	3/3811 (0.1%)
All	All	0.72	2/16635 (0.0%)	0.80	21/22653 (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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	GLU	CB-CG	-5.67	1.41	1.52
1	B	37	ALA	CA-CB	5.21	1.63	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	246	ALA	N-CA-C	-8.71	87.48	111.00
1	B	264	LEU	CA-CB-CG	7.80	133.24	115.30
1	E	197	LEU	CA-CB-CG	7.31	132.11	115.30
1	E	334	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	E	264	LEU	CA-CB-CG	6.91	131.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	330	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	C	264	LEU	CA-CB-CG	6.43	130.08	115.30
1	D	264	LEU	CA-CB-CG	6.26	129.70	115.30
1	D	71	LEU	CA-CB-CG	-5.98	101.55	115.30
1	E	16	VAL	CB-CA-C	-5.96	100.08	111.40
1	B	294	LEU	CA-CB-CG	5.79	128.62	115.30
1	D	185	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	F	334	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	D	185	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	71	LEU	CA-CB-CG	-5.59	102.44	115.30
1	D	294	LEU	CA-CB-CG	5.52	128.00	115.30
1	F	334	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	70	LEU	CB-CG-CD2	5.29	119.99	111.00
1	C	234	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	84	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	71	LEU	CB-CG-CD1	5.06	119.60	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	245	LYS	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	2727	0	2756	43	0
1	B	2707	0	2716	25	0
1	C	2682	0	2689	28	0
1	D	2712	0	2734	25	0
1	E	2742	0	2751	24	0
1	F	2742	0	2751	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	3	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	3	0	0
3	C	6	0	3	0	0
3	D	6	0	3	0	0
3	E	6	0	3	5	0
3	F	6	0	3	6	0
4	E	44	0	26	5	0
4	F	44	0	26	7	0
5	A	184	0	0	2	0
5	B	228	0	0	3	0
5	C	185	0	0	1	0
5	D	232	0	0	1	0
5	E	195	0	0	2	0
5	F	252	0	0	3	0
All	All	17715	0	16467	167	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 (167) 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:A:75:LYS:NZ	3:A:1373:PYR:H32	1.75	1.00
3:F:1375:PYR:H32	4:F:1376:NAD:C5N	1.93	0.99
3:E:1374:PYR:H32	4:E:1375:NAD:C5N	1.96	0.95
1:F:282:THR:HG22	1:F:285:HIS:H	1.39	0.86
1:D:267:ILE:HG22	1:D:267:ILE:O	1.75	0.86
3:E:1374:PYR:H32	4:E:1375:NAD:C4N	2.08	0.84
1:A:269:ILE:HG13	1:A:297:CYS:HB3	1.58	0.84
1:A:75:LYS:NZ	3:A:1373:PYR:C3	2.41	0.82
1:C:281:THR:HG21	1:C:286:PRO:O	1.80	0.80
1:E:240:LEU:HG	4:E:1375:NAD:H3D	1.64	0.79
1:B:255:VAL:HG11	1:B:290:VAL:HG22	1.66	0.76
1:A:75:LYS:HZ3	3:A:1373:PYR:H32	1.46	0.76
1:B:101:ARG:NH1	1:B:359:LEU:O	2.20	0.74
1:A:75:LYS:HZ2	3:A:1373:PYR:H32	1.50	0.73
1:A:353:GLU:O	1:A:357:THR:HG23	1.88	0.73
1:B:113:THR:OG1	1:B:346:HIS:HD2	1.71	0.73
1:D:255:VAL:HG11	1:D:290:VAL:HG22	1.72	0.72
1:A:75:LYS:HZ3	3:A:1373:PYR:C3	2.03	0.71
1:B:353:GLU:O	1:B:357:THR:HG23	1.91	0.70
1:C:330:ARG:HD3	1:C:334:ARG:NH2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:NH1	1:A:359:LEU:O	2.26	0.69
1:C:222:ALA:O	1:C:226:GLU:HG3	1.95	0.67
3:F:1375:PYR:H32	4:F:1376:NAD:C4N	2.25	0.66
1:F:282:THR:HG23	1:F:284:ASP:H	1.61	0.66
1:A:96:HIS:NE2	3:A:1373:PYR:H31	2.10	0.65
1:E:255:VAL:HG11	1:E:290:VAL:HG22	1.78	0.65
3:E:1374:PYR:C3	4:E:1375:NAD:C4N	2.75	0.65
1:E:282:THR:HG22	1:E:285:HIS:H	1.62	0.65
3:F:1375:PYR:C3	4:F:1376:NAD:C5N	2.72	0.64
1:B:62:ASP:OD1	1:B:84:ARG:HD3	1.96	0.64
1:B:87:HIS:CE1	1:B:347:GLU:HG2	2.31	0.64
1:D:244:ALA:O	1:D:245:LYS:HB3	1.98	0.64
1:D:318[B]:MET:HG2	5:D:2198:HOH:O	1.98	0.64
1:A:329:TRP:H	1:A:330[A]:ARG:HH21	1.48	0.62
1:D:113:THR:OG1	1:D:346:HIS:HD2	1.83	0.62
1:E:2:ARG:HG2	1:E:32:GLU:HB2	1.82	0.62
1:E:60:THR:HG22	1:E:62:ASP:H	1.64	0.62
1:A:255:VAL:HG11	1:A:290:VAL:HG22	1.83	0.60
1:A:214:ARG:HG3	1:B:214:ARG:HG3	1.84	0.60
1:A:58:VAL:HG21	1:A:64:VAL:HG22	1.84	0.59
1:D:240:LEU:HD23	1:D:271:GLN:HE22	1.67	0.58
1:B:87:HIS:HE1	1:B:347:GLU:HG2	1.69	0.58
3:E:1374:PYR:C3	4:E:1375:NAD:C5N	2.77	0.58
1:A:247:PRO:HG2	1:A:249:LEU:HD11	1.87	0.57
1:B:188:ASN:HD21	1:B:214:ARG:HD3	1.72	0.55
1:C:63:GLN:NE2	5:C:2036:HOH:O	2.38	0.55
1:D:222:ALA:O	1:D:226:GLU:HG3	2.07	0.55
1:D:267:ILE:O	1:D:267:ILE:CG2	2.47	0.54
1:F:330:ARG:HD2	5:F:2212:HOH:O	2.07	0.54
1:A:58:VAL:HG21	1:A:64:VAL:CG2	2.37	0.54
1:E:20:PRO:HA	1:E:23:VAL:HG13	1.90	0.54
1:A:329:TRP:H	1:A:330[A]:ARG:NH2	2.06	0.54
1:D:290:VAL:HG13	1:D:295:PHE:CD1	2.42	0.54
1:B:296:TYR:CZ	1:B:298:VAL:HG13	2.43	0.54
3:F:1375:PYR:C3	4:F:1376:NAD:C4N	2.86	0.53
1:E:290:VAL:HG13	1:E:295:PHE:CD1	2.43	0.53
1:B:296:TYR:CE2	1:B:298:VAL:HG13	2.43	0.53
1:C:281:THR:HG23	1:C:286:PRO:HA	1.90	0.53
1:B:290:VAL:HG13	1:B:295:PHE:CD1	2.43	0.53
1:C:281:THR:CG2	1:C:298:VAL:HG12	2.39	0.53
1:A:283:TYR:CD1	1:C:152:THR:HG21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:THR:HG23	1:E:284:ASP:H	1.75	0.52
1:B:330:ARG:HG3	5:B:2215:HOH:O	2.09	0.52
1:F:214:ARG:NH2	5:F:2141:HOH:O	2.38	0.52
1:F:290:VAL:O	1:F:293:THR:HB	2.10	0.52
1:B:96:HIS:HD2	5:B:2061:HOH:O	1.93	0.52
1:C:255:VAL:HG11	1:C:290:VAL:HG22	1.91	0.52
1:A:58:VAL:CG2	1:A:64:VAL:CG2	2.88	0.51
1:A:249:LEU:N	1:A:249:LEU:HD12	2.26	0.51
1:A:62:ASP:HB3	1:A:84:ARG:HD3	1.91	0.51
1:C:330:ARG:HD3	1:C:334:ARG:HH22	1.74	0.51
1:E:60:THR:HG22	1:E:62:ASP:N	2.26	0.51
1:D:282:THR:HG22	1:D:284:ASP:N	2.26	0.50
1:E:361:VAL:HG13	1:E:362:PRO:HD2	1.93	0.50
1:B:188:ASN:HD21	1:B:214:ARG:CD	2.24	0.50
1:E:156:ARG:O	1:F:307:LYS:HE3	2.11	0.50
1:C:290:VAL:HG13	1:C:295:PHE:CD1	2.47	0.50
1:C:23:VAL:HG22	1:C:53:ALA:HB1	1.92	0.50
1:D:282:THR:HG22	1:D:284:ASP:H	1.77	0.50
1:E:51:LYS:HD2	1:E:57:LEU:HD12	1.94	0.50
1:A:287:THR:HB	1:A:294:LEU:HD22	1.93	0.50
1:A:330[A]:ARG:H	1:A:330[A]:ARG:NE	2.09	0.50
1:D:239:VAL:HG21	1:D:249:LEU:HD22	1.93	0.50
1:E:282:THR:CG2	1:E:284:ASP:H	2.24	0.49
1:A:58:VAL:CG2	1:A:64:VAL:HG22	2.42	0.49
1:E:214:ARG:NH2	5:E:2110:HOH:O	2.34	0.49
1:F:334:ARG:HD2	1:F:370:LEU:O	2.11	0.49
1:D:250:VAL:HG13	1:D:254:LEU:HD23	1.95	0.48
3:F:1375:PYR:H32	4:F:1376:NAD:H5N	1.88	0.48
1:C:23:VAL:HG22	1:C:53:ALA:CB	2.43	0.48
1:F:329:TRP:HH2	1:F:369:VAL:HG13	1.78	0.47
1:C:356:ALA:CB	1:C:363:PHE:HB2	2.44	0.47
1:D:269:ILE:C	1:D:271:GLN:H	2.18	0.47
1:F:264:LEU:HD13	1:F:293:THR:CG2	2.45	0.47
1:A:329:TRP:CE2	1:A:330[A]:ARG:HG3	2.49	0.47
1:F:330:ARG:HD3	1:F:334:ARG:CZ	2.45	0.47
1:A:331:ALA:HA	1:A:334[B]:ARG:HD3	1.97	0.47
1:C:149:LEU:HA	1:C:149:LEU:HD23	1.79	0.47
1:A:249:LEU:N	1:A:249:LEU:CD1	2.78	0.47
1:D:65:TRP:CD1	1:D:84:ARG:HD3	2.49	0.47
1:B:255:VAL:HG11	1:B:290:VAL:CG2	2.41	0.47
1:C:202:ASP:O	1:C:206:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG21	1:C:283:TYR:CD1	2.51	0.46
1:B:284:ASP:OD1	1:B:284:ASP:N	2.38	0.46
1:E:282:THR:CG2	1:E:284:ASP:HB2	2.45	0.46
1:A:87:HIS:NE2	1:A:347:GLU:HG2	2.29	0.46
1:C:281:THR:HG22	1:C:298:VAL:HA	1.98	0.46
1:E:366:PRO:HD2	5:E:2187:HOH:O	2.16	0.45
1:E:20:PRO:HA	1:E:23:VAL:CG1	2.45	0.45
1:D:247:PRO:HB2	1:D:249:LEU:CD1	2.47	0.45
1:F:244:ALA:HB2	1:F:354:ARG:HG2	1.99	0.45
1:D:239:VAL:HG21	1:D:249:LEU:CD2	2.46	0.45
1:C:284:ASP:N	1:C:284:ASP:OD1	2.48	0.45
1:D:25:GLU:O	1:D:29:ARG:HG3	2.16	0.45
1:C:346:HIS:CD2	1:C:369:VAL:HG11	2.52	0.45
1:F:211:PHE:CD1	1:F:215:ILE:HD12	2.52	0.44
1:D:248:LYS:HD3	1:D:276:GLU:HA	1.99	0.44
1:C:267:ILE:HA	1:C:301:MET:HE1	2.00	0.44
1:C:73:LYS:HE3	1:C:75:LYS:O	2.18	0.44
1:D:85:LEU:HD13	1:D:107:LEU:HD23	1.99	0.44
1:F:365:GLU:HG3	5:F:2242:HOH:O	2.18	0.44
1:C:353:GLU:O	1:C:357:THR:HG23	2.18	0.44
1:A:75:LYS:NZ	3:A:1373:PYR:H33	2.30	0.44
1:A:329:TRP:N	1:A:330[A]:ARG:HH21	2.14	0.44
1:E:19:THR:HB	1:E:20:PRO:HD2	1.99	0.43
1:A:328:GLY:CA	1:A:330[A]:ARG:HH21	2.30	0.43
1:A:331:ALA:O	1:A:334[B]:ARG:HB2	2.18	0.43
1:C:264:LEU:HG	1:C:295:PHE:CE1	2.54	0.43
1:A:11:ASN:HD22	1:A:12:ASN:N	2.17	0.43
1:D:211:PHE:CD1	1:D:215:ILE:HD12	2.54	0.43
1:B:269:ILE:HD13	1:B:278:SER:HB3	2.00	0.43
1:A:87:HIS:CD2	1:A:347:GLU:HG2	2.53	0.43
1:B:283:TYR:CE1	1:B:304[A]:SER:OG	2.68	0.43
1:B:283:TYR:HE1	1:B:304[A]:SER:OG	2.02	0.43
1:A:186:ILE:O	1:A:190:MET:HG3	2.18	0.43
1:C:11:ASN:O	1:C:12:ASN:HB2	2.18	0.43
1:D:95:LEU:HD12	1:D:116:ALA:HB2	2.01	0.42
1:B:143:GLN:HG2	1:D:190:MET:CE	2.49	0.42
1:A:181:TYR:OH	1:A:210:GLU:OE1	2.32	0.42
1:E:47:ASP:HB3	1:E:57:LEU:HD13	2.00	0.42
1:B:283:TYR:CD1	1:D:152:THR:HG21	2.55	0.42
1:F:234:LEU:HD12	1:F:263:VAL:O	2.20	0.42
1:A:80:ALA:HB3	5:A:2005:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:HG	1:B:295:PHE:CE1	2.55	0.41
1:B:239:VAL:HG21	1:B:249:LEU:CD2	2.50	0.41
1:C:151:ARG:HD3	1:C:155:GLY:O	2.20	0.41
1:A:264:LEU:HG	1:A:295:PHE:CE1	2.55	0.41
1:B:14:PHE:CE2	5:B:2014:HOH:O	2.70	0.41
3:F:1375:PYR:C2	4:F:1376:NAD:C4N	2.98	0.41
1:A:283:TYR:CE1	1:A:304:SER:HB3	2.55	0.41
1:A:86:ARG:NH1	5:A:2050:HOH:O	2.53	0.41
1:A:140:LEU:HD11	1:A:305:VAL:HG22	2.03	0.41
1:E:175:GLY:O	1:E:180:GLY:HA3	2.20	0.41
1:F:10:LYS:HE3	1:F:76:GLU:OE2	2.21	0.41
1:E:65:TRP:CD1	1:E:84:ARG:HD3	2.56	0.41
1:A:296:TYR:CZ	1:A:298:VAL:HG13	2.56	0.41
1:F:267:ILE:O	4:F:1376:NAD:H2N	2.21	0.41
1:D:287:THR:HA	1:D:295:PHE:O	2.21	0.41
1:C:23:VAL:CG2	1:C:53:ALA:CB	2.99	0.41
1:F:329:TRP:CH2	1:F:369:VAL:HG13	2.56	0.41
1:F:264:LEU:CD1	1:F:293:THR:HG23	2.51	0.40
1:E:104:THR:HG22	1:E:108:LEU:HD22	2.02	0.40
1:C:23:VAL:CG2	1:C:53:ALA:HB3	2.52	0.40
1:E:75:LYS:NZ	3:E:1374:PYR:O3	2.53	0.40
1:E:157:GLY:O	1:F:307:LYS:HB2	2.22	0.40
1:C:151:ARG:HA	1:C:151:ARG:HD3	1.65	0.40
1:A:240:LEU:C	1:A:240:LEU:HD23	2.42	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	368/377 (98%)	360 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	365/377 (97%)	358 (98%)	7 (2%)	0	100 100
1	C	361/377 (96%)	357 (99%)	4 (1%)	0	100 100
1	D	366/377 (97%)	358 (98%)	7 (2%)	1 (0%)	46 41
1	E	372/377 (99%)	366 (98%)	6 (2%)	0	100 100
1	F	372/377 (99%)	367 (99%)	5 (1%)	0	100 100
All	All	2204/2262 (97%)	2166 (98%)	37 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	245	LYS

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	279/282 (99%)	254 (91%)	25 (9%)	12 7
1	B	275/282 (98%)	259 (94%)	16 (6%)	25 19
1	C	273/282 (97%)	251 (92%)	22 (8%)	15 9
1	D	277/282 (98%)	261 (94%)	16 (6%)	25 19
1	E	279/282 (99%)	261 (94%)	18 (6%)	21 15
1	F	279/282 (99%)	270 (97%)	9 (3%)	46 44
All	All	1662/1692 (98%)	1556 (94%)	106 (6%)	23 15

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	50	PHE
1	A	60	THR
1	A	62	ASP
1	A	70	LEU

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Mol	Chain	Res	Type
1	A	71	LEU
1	A	86	ARG
1	A	87	HIS
1	A	185	ARG
1	A	212[A]	CYS
1	A	212[B]	CYS
1	A	234	LEU
1	A	241	VAL
1	A	264	LEU
1	A	269	ILE
1	A	293	THR
1	A	294	LEU
1	A	307	LYS
1	A	330[A]	ARG
1	A	330[B]	ARG
1	A	336	ASN
1	A	339	LEU
1	A	350	LEU
1	A	357	THR
1	A	369	VAL
1	B	2	ARG
1	B	86	ARG
1	B	87	HIS
1	B	249	LEU
1	B	264	LEU
1	B	271	GLN
1	B	293	THR
1	B	294	LEU
1	B	323	GLU
1	B	336	ASN
1	B	339	LEU
1	B	350	LEU
1	B	357	THR
1	B	368	SER
1	B	369	VAL
1	B	370	LEU
1	C	23	VAL
1	C	58	VAL
1	C	70	LEU
1	C	71	LEU
1	C	84	ARG
1	C	130	LEU

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Mol	Chain	Res	Type
1	C	144	VAL
1	C	151	ARG
1	C	212	CYS
1	C	220	SER
1	C	234	LEU
1	C	240	LEU
1	C	249	LEU
1	C	264	LEU
1	C	281	THR
1	C	284	ASP
1	C	290	VAL
1	C	293	THR
1	C	298	VAL
1	C	339	LEU
1	C	350	LEU
1	C	361	VAL
1	D	2	ARG
1	D	71	LEU
1	D	101	ARG
1	D	185	ARG
1	D	202	ASP
1	D	212[A]	CYS
1	D	212[B]	CYS
1	D	240	LEU
1	D	264	LEU
1	D	270	ASP
1	D	282	THR
1	D	290	VAL
1	D	293	THR
1	D	294	LEU
1	D	368	SER
1	D	369	VAL
1	E	3	VAL
1	E	16	VAL
1	E	23	VAL
1	E	70	LEU
1	E	71	LEU
1	E	108	LEU
1	E	144	VAL
1	E	197	LEU
1	E	212[A]	CYS
1	E	212[B]	CYS

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Mol	Chain	Res	Type
1	E	240	LEU
1	E	254	LEU
1	E	264	LEU
1	E	282	THR
1	E	339	LEU
1	E	350	LEU
1	E	365	GLU
1	E	369	VAL
1	F	58	VAL
1	F	71	LEU
1	F	212[A]	CYS
1	F	212[B]	CYS
1	F	254	LEU
1	F	282	THR
1	F	293	THR
1	F	307	LYS
1	F	369	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	63	GLN
1	A	121	GLN
1	A	143	GLN
1	A	300	ASN
1	A	315	ASN
1	A	336	ASN
1	B	96	HIS
1	B	188	ASN
1	B	336	ASN
1	B	346	HIS
1	C	63	GLN
1	C	216	HIS
1	D	121	GLN
1	D	143	GLN
1	D	300	ASN
1	D	346	HIS
1	E	148	HIS
1	E	206	GLN
1	E	373	HIS
1	F	373	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PYR	A	1373	-	2,5,5	1.55	1 (50%)	2,6,6	0.38	0
3	PYR	B	1373	-	2,5,5	1.63	1 (50%)	2,6,6	0.35	0
3	PYR	C	1371	-	2,5,5	1.74	1 (50%)	2,6,6	0.36	0
3	PYR	D	1371	-	2,5,5	1.92	1 (50%)	2,6,6	0.97	0
3	PYR	E	1374	-	2,5,5	1.30	0	2,6,6	1.10	0
4	NAD	E	1375	-	38,48,48	1.63	3 (7%)	47,73,73	2.27	6 (12%)
3	PYR	F	1375	-	2,5,5	1.49	1 (50%)	2,6,6	0.85	0
4	NAD	F	1376	-	38,48,48	1.70	3 (7%)	47,73,73	2.57	10 (21%)

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
3	PYR	A	1373	-	-	0/0/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PYR	B	1373	-	-	0/0/4/4	0/0/0/0
3	PYR	C	1371	-	-	0/0/4/4	0/0/0/0
3	PYR	D	1371	-	-	0/0/4/4	0/0/0/0
3	PYR	E	1374	-	-	0/0/4/4	0/0/0/0
4	NAD	E	1375	-	-	0/22/62/62	0/5/5/5
3	PYR	F	1375	-	-	0/0/4/4	0/0/0/0
4	NAD	F	1376	-	-	0/22/62/62	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1375	PYR	O3-C2	2.09	1.30	1.22
3	A	1373	PYR	O3-C2	2.19	1.30	1.22
3	B	1373	PYR	O3-C2	2.30	1.30	1.22
3	C	1371	PYR	O3-C2	2.46	1.31	1.22
3	D	1371	PYR	O3-C2	2.71	1.32	1.22
4	E	1375	NAD	C2A-N1A	3.43	1.40	1.33
4	E	1375	NAD	C2A-N3A	3.77	1.38	1.32
4	F	1376	NAD	C2A-N1A	3.91	1.41	1.33
4	F	1376	NAD	C2A-N3A	4.79	1.40	1.32
4	F	1376	NAD	O7N-C7N	6.70	1.38	1.24
4	E	1375	NAD	O7N-C7N	7.34	1.39	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1376	NAD	N3A-C2A-N1A	-10.62	120.77	128.89
4	E	1375	NAD	N3A-C2A-N1A	-10.23	121.06	128.89
4	E	1375	NAD	C4B-O4B-C1B	-4.23	105.07	109.72
4	F	1376	NAD	O7N-C7N-C3N	-3.83	115.40	119.59
4	F	1376	NAD	C4B-O4B-C1B	-3.34	106.05	109.72
4	F	1376	NAD	C2B-C1B-N9A	-3.05	109.62	114.29
4	E	1375	NAD	C4D-O4D-C1D	-2.54	106.93	109.72
4	F	1376	NAD	C4D-O4D-C1D	-2.49	106.98	109.72
4	F	1376	NAD	C1B-N9A-C4A	-2.20	123.63	126.94
4	E	1375	NAD	PN-O3-PA	-2.03	127.02	132.73
4	F	1376	NAD	O7N-C7N-N7N	-2.03	119.73	122.59
4	F	1376	NAD	O2A-PA-O3	2.05	114.38	105.09
4	E	1375	NAD	C3N-C7N-N7N	2.95	121.04	117.82
4	F	1376	NAD	C3N-C7N-N7N	6.44	124.86	117.82
4	E	1375	NAD	O4D-C1D-N1N	8.05	116.97	108.13
4	F	1376	NAD	O4D-C1D-N1N	8.47	117.43	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1373	PYR	7	0
3	E	1374	PYR	5	0
4	E	1375	NAD	5	0
3	F	1375	PYR	6	0
4	F	1376	NAD	7	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, 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	368/377 (97%)	0.26	9 (2%)	62	63	3, 17, 29, 42	0
1	B	368/377 (97%)	0.09	10 (2%)	58	58	3, 14, 27, 44	0
1	C	365/377 (96%)	0.22	16 (4%)	38	39	4, 16, 33, 37	0
1	D	367/377 (97%)	0.06	6 (1%)	74	75	3, 14, 28, 46	0
1	E	373/377 (98%)	0.33	10 (2%)	58	58	6, 20, 31, 57	0
1	F	373/377 (98%)	0.16	3 (0%)	87	88	6, 15, 23, 53	0
All	All	2214/2262 (97%)	0.19	54 (2%)	62	63	3, 16, 29, 57	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	GLY	4.6
1	E	372	HIS	4.0
1	A	371	ALA	3.9
1	F	373	HIS	3.8
1	C	283	TYR	3.8
1	E	373	HIS	3.6
1	F	372	HIS	3.4
1	E	83	GLY	3.3
1	C	363	PHE	3.3
1	A	283	TYR	3.3
1	C	368	SER	3.1
1	A	14	PHE	3.0
1	B	240	LEU	3.0
1	B	363	PHE	2.9
1	A	370	LEU	2.9
1	E	68	ALA	2.9
1	B	369	VAL	2.9
1	C	361	VAL	2.9
1	C	246	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	244	ALA	2.8
1	B	370	LEU	2.8
1	C	362	PRO	2.8
1	B	367	ALA	2.6
1	A	270	ASP	2.6
1	C	356	ALA	2.6
1	C	367	ALA	2.6
1	D	367	ALA	2.5
1	D	270	ASP	2.5
1	A	51	LYS	2.4
1	B	365	GLU	2.4
1	C	292	ASP	2.3
1	B	283	TYR	2.3
1	A	368	SER	2.3
1	B	347	GLU	2.3
1	E	186	ILE	2.3
1	C	357	THR	2.3
1	D	240	LEU	2.3
1	E	79	ALA	2.2
1	F	194	VAL	2.2
1	E	215	ILE	2.2
1	A	369	VAL	2.2
1	D	245	LYS	2.2
1	E	34	LEU	2.1
1	A	62	ASP	2.1
1	B	368	SER	2.1
1	C	354	ARG	2.1
1	D	369	VAL	2.1
1	C	358	ASP	2.1
1	C	359	LEU	2.1
1	E	56	GLN	2.1
1	D	368	SER	2.0
1	E	48	ALA	2.0
1	C	284	ASP	2.0
1	C	365	GLU	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
3	PYR	F	1375	6/6	0.92	0.27	6.66	18,23,28,32	0
3	PYR	D	1371	6/6	0.84	0.28	5.93	39,42,45,47	0
3	PYR	E	1374	6/6	0.91	0.25	5.76	34,37,40,43	0
3	PYR	B	1373	6/6	0.87	0.18	3.62	32,38,39,39	0
3	PYR	C	1371	6/6	0.88	0.18	3.19	37,40,42,43	0
3	PYR	A	1373	6/6	0.82	0.24	1.87	34,38,39,39	0
4	NAD	E	1375	44/44	0.98	0.11	-0.58	8,13,20,22	0
4	NAD	F	1376	44/44	0.98	0.11	-0.91	3,7,11,15	0
2	MG	A	1372	1/1	0.73	0.27	-	32,32,32,32	0
2	MG	F	1374	1/1	0.59	0.15	-	53,53,53,53	0
2	MG	B	1372	1/1	0.94	0.32	-	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.