Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:35 PM GMT

PDB ID	:	4YR9
Title	:	mouse TDH with NAD+ bound
Authors	:	He, C.; Li, F.
Deposited on	:	2015-03-14
Resolution	:	2.80 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:

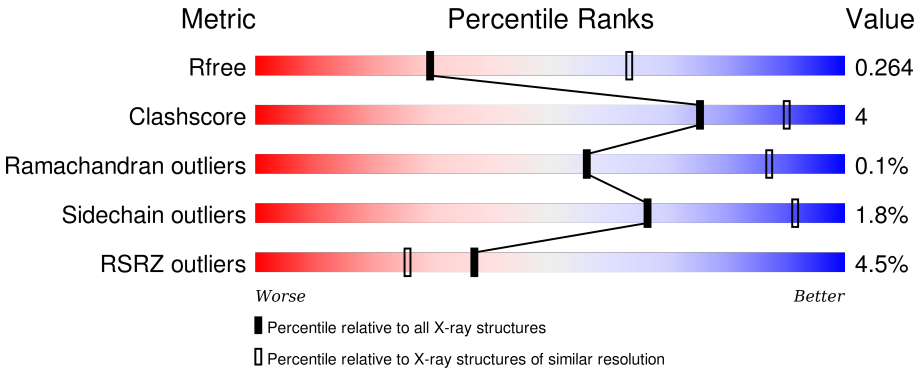
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	329	84% 9% • 6%
1	B	329	3% 80% 13% 7%
1	C	329	2% 83% 10% 7%
1	D	329	4% 82% 12% 6%
1	E	329	5% 83% 11% 6%

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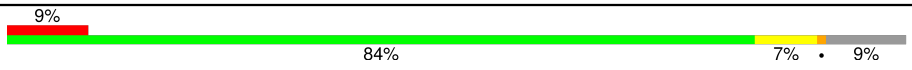
Mol	Chain	Length	Quality of chain
1	F	329	

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	GOL	A	1002	-	-	-	X
3	GOL	B	1002	-	-	-	X
3	GOL	C	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14852 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.

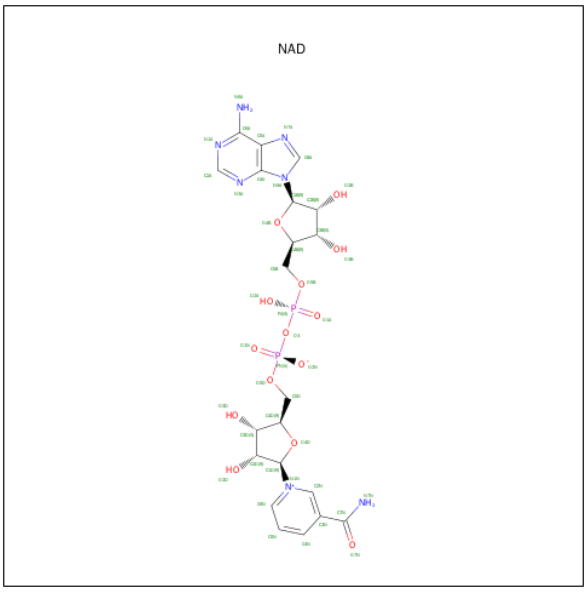
- Molecule 1 is a protein called L-threonine 3-dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2430	1555	424	438	13			
1	B	307	Total	C	N	O	S	0	0	0
			2420	1549	422	436	13			
1	C	307	Total	C	N	O	S	0	0	0
			2415	1545	420	437	13			
1	D	308	Total	C	N	O	S	0	0	0
			2423	1551	423	436	13			
1	E	308	Total	C	N	O	S	0	0	0
			2430	1555	424	438	13			
1	F	301	Total	C	N	O	S	0	0	0
			2377	1521	413	430	13			

There are 12 discrepancies between the modelled and reference sequences:

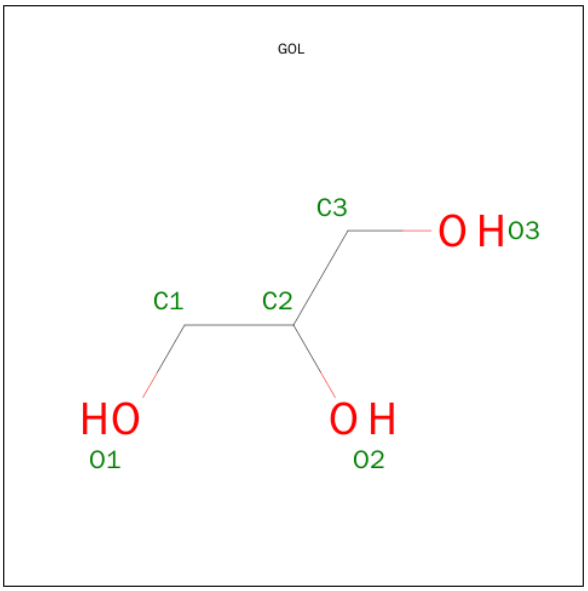
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	HIS	-	expression tag	UNP Q8K3F7
A	46	MET	-	expression tag	UNP Q8K3F7
B	45	HIS	-	expression tag	UNP Q8K3F7
B	46	MET	-	expression tag	UNP Q8K3F7
C	45	HIS	-	expression tag	UNP Q8K3F7
C	46	MET	-	expression tag	UNP Q8K3F7
D	45	HIS	-	expression tag	UNP Q8K3F7
D	46	MET	-	expression tag	UNP Q8K3F7
E	45	HIS	-	expression tag	UNP Q8K3F7
E	46	MET	-	expression tag	UNP Q8K3F7
F	45	HIS	-	expression tag	UNP Q8K3F7
F	46	MET	-	expression tag	UNP Q8K3F7

- 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		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

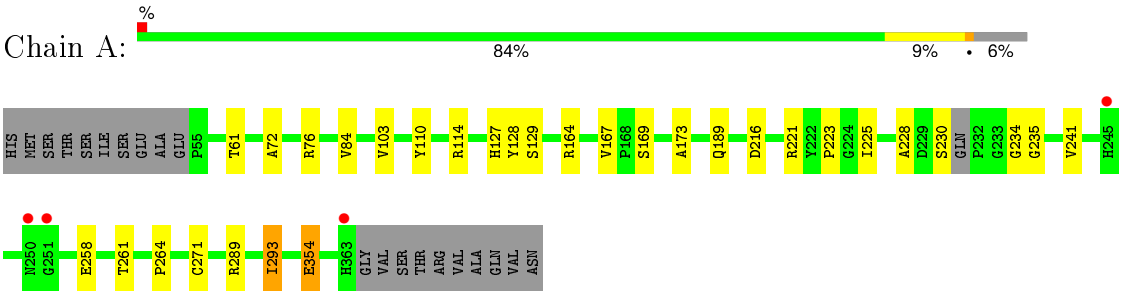
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	21	Total O 21 21	0	0
4	C	10	Total O 10 10	0	0
4	D	16	Total O 16 16	0	0
4	E	7	Total O 7 7	0	0
4	F	7	Total O 7 7	0	0

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.

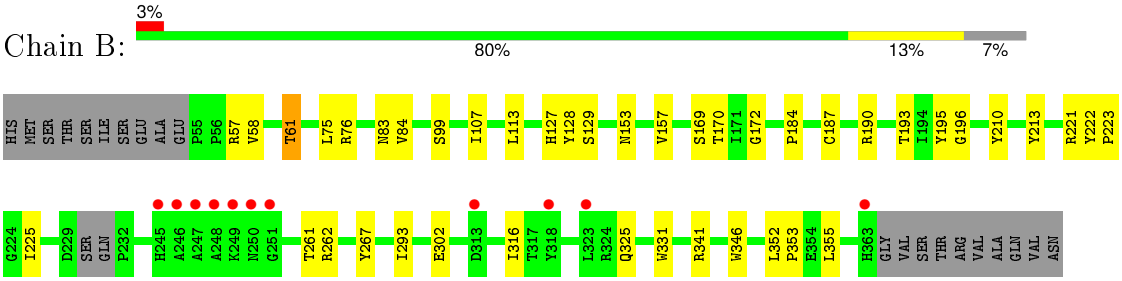
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain A:



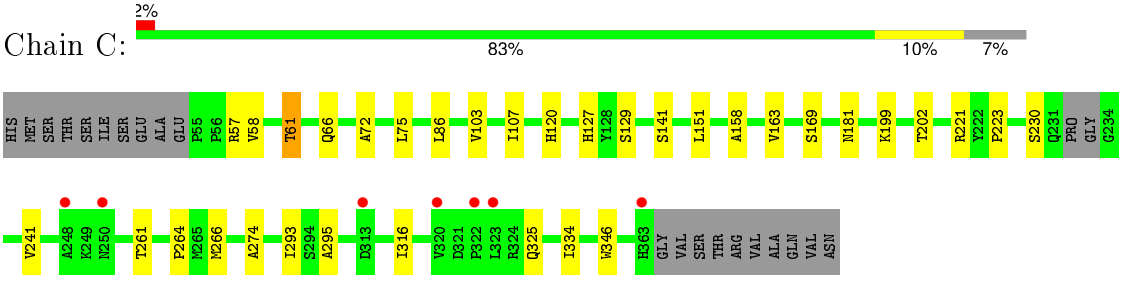
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain B:



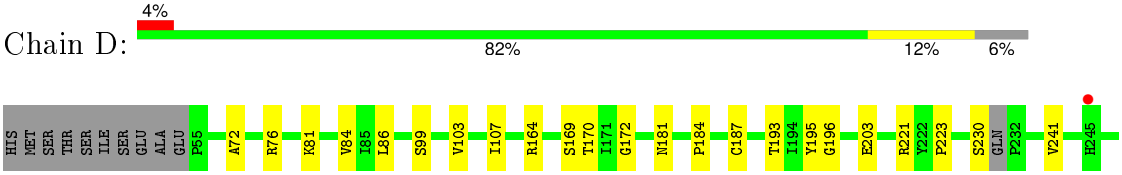
- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

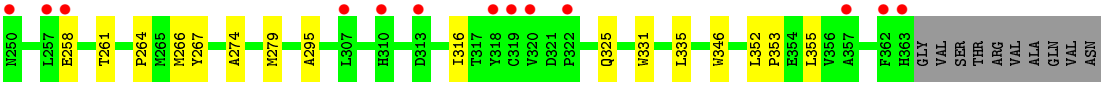
Chain C:



- Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

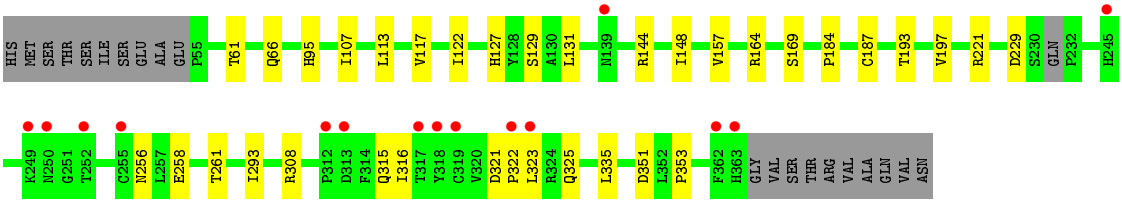
Chain D:





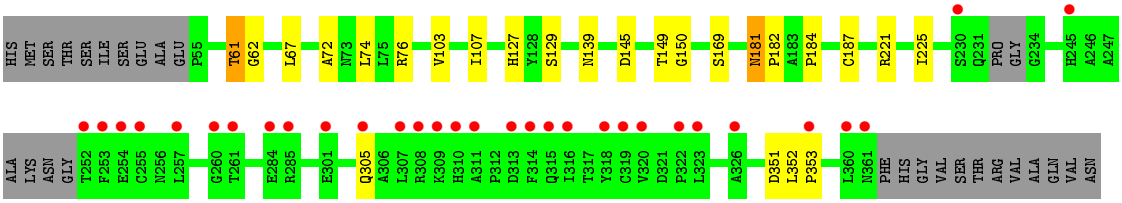
• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain E:



• Molecule 1: L-threonine 3-dehydrogenase, mitochondrial

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.15Å 160.13Å 194.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.42 – 2.80 36.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.4 (36.42-2.80) 92.4 (36.42-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.264 0.215 , 0.264	Depositor DCC
R_{free} test set	2700 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 53476 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14852	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: GOL, 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	0.29	0/2494	0.47	0/3391
1	B	0.29	0/2484	0.48	0/3379
1	C	0.29	0/2477	0.47	0/3370
1	D	0.29	0/2487	0.47	0/3383
1	E	0.28	0/2494	0.48	0/3391
1	F	0.29	0/2437	0.47	0/3314
All	All	0.29	0/14873	0.48	0/20228

There are no bond length outliers.

There are no bond angle outliers.

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	2430	0	2401	19	0
1	B	2420	0	2385	24	0
1	C	2415	0	2376	21	0
1	D	2423	0	2388	20	0
1	E	2430	0	2401	17	0
1	F	2377	0	2348	13	0
2	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	2	0
2	F	44	0	26	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	14	0	0	0	0
4	B	21	0	0	0	0
4	C	10	0	0	0	0
4	D	16	0	0	0	0
4	E	7	0	0	1	0
4	F	7	0	0	0	0
All	All	14852	0	14479	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (113) 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:E:61:THR:HG22	1:E:129:SER:HB3	1.67	0.76
1:C:261:THR:HG21	1:C:325:GLN:HE22	1.51	0.76
1:D:164:ARG:NH2	1:D:279:MET:O	2.27	0.68
1:D:169:SER:HB3	1:D:221:ARG:HG2	1.74	0.67
1:E:261:THR:HG21	1:E:325:GLN:HE22	1.57	0.67
1:A:169:SER:HB3	1:A:221:ARG:HG2	1.75	0.67
1:B:169:SER:HB3	1:B:221:ARG:HG2	1.75	0.67
1:C:230:SER:HB3	1:C:241:VAL:HG11	1.79	0.63
1:E:256:ASN:HB2	1:E:321:ASP:HB2	1.83	0.59
1:F:67:LEU:HD21	1:F:225:ILE:HG21	1.84	0.59
1:E:66:GLN:NE2	2:E:1001:NAD:H72N	1.99	0.59
1:A:223:PRO:HD3	1:A:293:ILE:HG23	1.86	0.57
1:E:169:SER:HB3	1:E:221:ARG:HG2	1.85	0.57
1:A:221:ARG:O	1:A:293:ILE:HG22	2.05	0.57
1:F:169:SER:HB3	1:F:221:ARG:HG2	1.86	0.56
1:E:351:ASP:HB3	1:E:353:PRO:HD2	1.86	0.56
1:C:72:ALA:HB2	1:C:86:LEU:HD13	1.87	0.55
1:F:62:GLY:HA3	1:F:129:SER:HB3	1.89	0.55
1:B:184:PRO:HG2	1:B:187:CYS:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:THR:HG21	1:C:127:HIS:ND1	2.21	0.54
1:C:169:SER:HB3	1:C:221:ARG:HG2	1.90	0.54
1:B:190:ARG:HH12	1:D:203:GLU:HB3	1.73	0.53
1:B:170:THR:HG21	1:B:195:TYR:CE2	2.44	0.53
1:E:184:PRO:HG2	1:E:187:CYS:HB3	1.89	0.52
1:B:341:ARG:HG2	1:B:346:TRP:O	2.09	0.52
1:D:261:THR:HG21	1:D:325:GLN:HE22	1.74	0.52
1:A:230:SER:HB3	1:A:241:VAL:HG11	1.92	0.52
1:F:61:THR:HG21	1:F:127:HIS:ND1	2.25	0.52
1:D:274:ALA:HB2	1:D:346:TRP:CZ3	2.45	0.51
1:D:352:LEU:HB3	1:D:353:PRO:HD3	1.92	0.51
1:D:266:MET:HE2	1:D:295:ALA:HB2	1.91	0.51
1:D:76:ARG:HG2	1:D:84:VAL:HB	1.91	0.51
1:B:61:THR:HG22	1:B:129:SER:H	1.76	0.50
1:B:107:ILE:HG12	1:B:127:HIS:HE1	1.76	0.49
1:B:172:GLY:HA2	1:B:331:TRP:NE1	2.28	0.48
1:D:170:THR:HG21	1:D:195:TYR:CE2	2.48	0.48
1:D:264:PRO:HG2	1:D:335:LEU:HD13	1.94	0.48
1:A:258:GLU:HB2	1:A:261:THR:HG23	1.94	0.48
1:C:158:ALA:HA	1:C:163:VAL:HB	1.94	0.48
1:D:267:TYR:HB2	1:D:355:LEU:HD13	1.96	0.48
1:F:107:ILE:HG22	1:F:150:GLY:HA2	1.95	0.47
1:E:322:PRO:HG2	1:E:323:LEU:HD12	1.96	0.47
1:C:223:PRO:HB3	1:C:264:PRO:HB2	1.97	0.47
1:A:61:THR:O	1:A:128:TYR:HB2	2.14	0.47
1:B:113:LEU:HB3	1:B:157:VAL:HG21	1.95	0.47
1:B:61:THR:HG21	1:B:127:HIS:ND1	2.29	0.47
1:C:181:ASN:HD22	1:C:334:ILE:HD12	1.80	0.47
1:D:81:LYS:HE3	1:D:99:SER:O	2.14	0.47
1:D:72:ALA:HB2	1:D:86:LEU:HD13	1.96	0.46
1:C:66:GLN:NE2	2:C:1001:NAD:H72N	2.13	0.46
1:E:193:THR:O	1:E:197:VAL:HG23	2.15	0.46
1:E:95:HIS:HB3	4:E:1103:HOH:O	2.14	0.46
1:D:230:SER:HB3	1:D:241:VAL:HG11	1.97	0.46
1:F:145:ASP:O	1:F:149:THR:HB	2.14	0.46
1:A:61:THR:HG21	1:A:127:HIS:ND1	2.31	0.46
1:D:184:PRO:HG2	1:D:187:CYS:HB3	1.99	0.45
1:F:352:LEU:HB3	1:F:353:PRO:HD3	1.97	0.45
1:A:225:ILE:HD12	1:A:271:CYS:HB2	1.97	0.45
1:A:223:PRO:HB3	1:A:264:PRO:HB2	1.99	0.45
1:B:222:TYR:HB3	1:B:225:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ARG:HD2	1:B:83:ASN:HD22	1.81	0.45
1:F:61:THR:HG22	1:F:129:SER:H	1.82	0.45
1:C:169:SER:HA	1:C:199:LYS:HD2	2.00	0.44
1:B:267:TYR:HB2	1:B:355:LEU:HD13	1.99	0.44
1:D:172:GLY:HA2	1:D:331:TRP:NE1	2.33	0.44
1:B:261:THR:HG21	1:B:325:GLN:HE22	1.82	0.44
1:C:61:THR:HG22	1:C:129:SER:H	1.83	0.44
1:C:266:MET:HE1	1:C:293:ILE:HG12	2.00	0.44
1:A:61:THR:HG22	1:A:129:SER:H	1.82	0.44
1:A:76:ARG:HG2	1:A:84:VAL:HB	2.00	0.43
1:C:107:ILE:HA	1:C:107:ILE:HD12	1.88	0.43
1:B:352:LEU:HB3	1:B:353:PRO:HD3	2.00	0.43
1:C:274:ALA:HB2	1:C:346:TRP:CZ3	2.54	0.43
1:B:153:ASN:O	1:B:157:VAL:HG23	2.19	0.43
1:F:184:PRO:HG2	1:F:187:CYS:HB3	2.00	0.43
1:E:144:ARG:HG3	1:E:148:ILE:HD12	2.01	0.43
1:E:129:SER:HB2	2:E:1001:NAD:N3A	2.34	0.43
1:A:354:GLU:H	1:A:354:GLU:HG2	1.59	0.43
1:D:193:THR:HG23	1:D:196:GLY:H	1.84	0.43
1:F:72:ALA:HB1	1:F:76:ARG:NH1	2.34	0.43
1:E:258:GLU:HB2	1:E:261:THR:HG23	2.01	0.43
1:B:61:THR:O	1:B:128:TYR:HB2	2.19	0.43
1:A:127:HIS:HB3	1:A:167:VAL:HG22	2.00	0.43
1:C:221:ARG:O	1:C:293:ILE:HG22	2.19	0.43
1:A:164:ARG:HG3	1:A:216:ASP:CG	2.40	0.42
1:E:113:LEU:HB3	1:E:157:VAL:HG21	2.01	0.42
1:A:234:GLY:HA3	1:A:235:GLY:HA3	1.72	0.42
1:C:151:LEU:HD21	1:C:202:THR:HA	2.01	0.42
1:A:173:ALA:O	1:A:189:GLN:NE2	2.51	0.42
1:F:72:ALA:HB1	1:F:76:ARG:HH11	1.85	0.42
1:D:258:GLU:HB2	1:D:261:THR:HG23	2.01	0.42
1:B:210:TYR:O	1:B:213:TYR:O	2.38	0.42
1:C:58:VAL:HG11	1:C:75:LEU:HD13	2.01	0.42
1:E:107:ILE:HG12	1:E:127:HIS:HE1	1.84	0.41
1:A:72:ALA:O	1:A:76:ARG:HG3	2.20	0.41
1:C:181:ASN:ND2	1:C:334:ILE:HD12	2.35	0.41
1:B:58:VAL:HG11	1:B:75:LEU:HD13	2.02	0.41
1:B:107:ILE:HD12	1:B:107:ILE:HA	1.93	0.41
1:B:76:ARG:HG3	1:B:84:VAL:HB	2.01	0.41
1:A:110:TYR:CE2	1:A:114:ARG:HD2	2.55	0.41
1:E:308:ARG:HH21	1:E:315:GLN:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ARG:HD2	1:A:289:ARG:HA	1.94	0.41
1:C:266:MET:HE3	1:C:295:ALA:HB2	2.01	0.41
1:F:107:ILE:HG22	1:F:150:GLY:CA	2.50	0.41
1:D:107:ILE:HD12	1:D:107:ILE:HA	1.81	0.41
1:B:262:ARG:NH2	1:B:302:GLU:OE2	2.54	0.41
1:D:223:PRO:HB3	1:D:264:PRO:HB2	2.02	0.41
1:C:57:ARG:NH1	1:C:120:HIS:O	2.51	0.41
1:E:117:VAL:HG13	1:E:122:ILE:HB	2.02	0.41
1:B:193:THR:HG23	1:B:196:GLY:H	1.86	0.40
1:B:223:PRO:O	1:B:225:ILE:HG13	2.21	0.40
1:F:181:ASN:HA	1:F:182:PRO:HA	1.89	0.40
1:C:261:THR:HG21	1:C:325:GLN:NE2	2.28	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	304/329 (92%)	294 (97%)	9 (3%)	1 (0%)	46 79
1	B	303/329 (92%)	292 (96%)	11 (4%)	0	100 100
1	C	303/329 (92%)	292 (96%)	11 (4%)	0	100 100
1	D	304/329 (92%)	288 (95%)	16 (5%)	0	100 100
1	E	304/329 (92%)	291 (96%)	13 (4%)	0	100 100
1	F	295/329 (90%)	280 (95%)	15 (5%)	0	100 100
All	All	1813/1974 (92%)	1737 (96%)	75 (4%)	1 (0%)	56 87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	ALA

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	259/277 (94%)	256 (99%)	3 (1%)	78 95
1	B	257/277 (93%)	253 (98%)	4 (2%)	70 93
1	C	256/277 (92%)	252 (98%)	4 (2%)	70 93
1	D	257/277 (93%)	254 (99%)	3 (1%)	78 95
1	E	259/277 (94%)	253 (98%)	6 (2%)	58 88
1	F	254/277 (92%)	247 (97%)	7 (3%)	51 84
All	All	1542/1662 (93%)	1515 (98%)	27 (2%)	66 91

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	A	293	ILE
1	A	354	GLU
1	B	61	THR
1	B	99	SER
1	B	293	ILE
1	B	316	ILE
1	C	61	THR
1	C	103	VAL
1	C	141	SER
1	C	316	ILE
1	D	103	VAL
1	D	181	ASN
1	D	316	ILE
1	E	131	LEU
1	E	164	ARG
1	E	229	ASP
1	E	293	ILE
1	E	316	ILE
1	E	335	LEU
1	F	61	THR
1	F	74	LEU

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Mol	Chain	Res	Type
1	F	103	VAL
1	F	139	ASN
1	F	181	ASN
1	F	305	GLN
1	F	351	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	83	ASN
1	A	153	ASN
1	B	66	GLN
1	B	83	ASN
1	B	120	HIS
1	B	153	ASN
1	B	325	GLN
1	C	66	GLN
1	C	95	HIS
1	C	153	ASN
1	C	181	ASN
1	D	66	GLN
1	D	83	ASN
1	D	153	ASN
1	D	325	GLN
1	E	66	GLN
1	E	127	HIS
1	E	139	ASN
1	E	153	ASN
1	E	325	GLN
1	F	66	GLN
1	F	153	ASN
1	F	305	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1001	-	42,48,48	0.83	1 (2%)	46,73,73	1.72	5 (10%)
3	GOL	A	1002	-	5,5,5	0.31	0	5,5,5	0.41	0
2	NAD	B	1001	-	42,48,48	0.86	1 (2%)	46,73,73	1.59	4 (8%)
3	GOL	B	1002	-	5,5,5	0.28	0	5,5,5	0.22	0
2	NAD	C	1001	-	42,48,48	0.81	1 (2%)	46,73,73	1.54	3 (6%)
3	GOL	C	1002	-	5,5,5	0.25	0	5,5,5	0.22	0
2	NAD	D	1001	-	42,48,48	0.85	1 (2%)	46,73,73	1.58	5 (10%)
2	NAD	E	1001	-	42,48,48	0.81	1 (2%)	46,73,73	1.57	5 (10%)
2	NAD	F	1001	-	42,48,48	0.81	1 (2%)	46,73,73	1.48	4 (8%)

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	1001	-	-	0/22/62/62	0/5/5/5
3	GOL	A	1002	-	-	0/4/4/4	0/0/0/0
2	NAD	B	1001	-	-	0/22/62/62	0/5/5/5
3	GOL	B	1002	-	-	0/4/4/4	0/0/0/0
2	NAD	C	1001	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	1002	-	-	0/4/4/4	0/0/0/0
2	NAD	D	1001	-	-	0/22/62/62	0/5/5/5
2	NAD	E	1001	-	-	0/22/62/62	0/5/5/5
2	NAD	F	1001	-	-	0/22/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	NAD	C5A-C4A	3.05	1.47	1.40
2	F	1001	NAD	C5A-C4A	3.05	1.47	1.40
2	D	1001	NAD	C5A-C4A	3.08	1.47	1.40
2	E	1001	NAD	C5A-C4A	3.08	1.47	1.40
2	C	1001	NAD	C5A-C4A	3.08	1.47	1.40
2	B	1001	NAD	C5A-C4A	3.20	1.47	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	NAD	N3A-C2A-N1A	-7.50	122.98	128.87
2	C	1001	NAD	N3A-C2A-N1A	-7.41	123.05	128.87
2	F	1001	NAD	N3A-C2A-N1A	-7.14	123.26	128.87
2	A	1001	NAD	N3A-C2A-N1A	-7.11	123.28	128.87
2	E	1001	NAD	N3A-C2A-N1A	-7.10	123.29	128.87
2	D	1001	NAD	N3A-C2A-N1A	-7.02	123.36	128.87
2	A	1001	NAD	C1B-N9A-C4A	-3.72	122.65	126.81
2	A	1001	NAD	C4B-O4B-C1B	-2.75	106.73	109.64
2	D	1001	NAD	C4B-O4B-C1B	-2.51	106.98	109.64
2	E	1001	NAD	C1B-N9A-C4A	-2.40	124.13	126.81
2	E	1001	NAD	C4B-O4B-C1B	-2.33	107.17	109.64
2	B	1001	NAD	C1B-N9A-C4A	-2.19	124.36	126.81
2	F	1001	NAD	C1B-N9A-C4A	-2.18	124.37	126.81
2	D	1001	NAD	C1B-N9A-C4A	-2.16	124.40	126.81
2	F	1001	NAD	O4B-C1B-N9A	2.01	111.91	108.11
2	B	1001	NAD	O4B-C1B-N9A	2.03	111.95	108.11
2	C	1001	NAD	O4D-C1D-N1N	2.30	110.59	108.10
2	E	1001	NAD	O4B-C1B-N9A	2.37	112.58	108.11
2	D	1001	NAD	O4B-C1B-N9A	3.25	114.25	108.11
2	A	1001	NAD	O4B-C1B-N9A	3.34	114.41	108.11
2	F	1001	NAD	O4D-C1D-N1N	3.63	112.03	108.10
2	C	1001	NAD	O4B-C1B-N9A	3.88	115.44	108.11
2	E	1001	NAD	O4D-C1D-N1N	4.04	112.46	108.10
2	B	1001	NAD	O4D-C1D-N1N	4.34	112.80	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	NAD	O4D-C1D-N1N	4.42	112.87	108.10
2	A	1001	NAD	O4D-C1D-N1N	5.18	113.70	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	NAD	1	0
2	E	1001	NAD	2	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	308/329 (93%)	-0.23	4 (1%) 79 71	21, 34, 57, 71	0
1	B	307/329 (93%)	-0.02	11 (3%) 46 34	24, 37, 74, 110	0
1	C	307/329 (93%)	-0.10	7 (2%) 64 52	23, 38, 83, 104	0
1	D	308/329 (93%)	0.15	14 (4%) 37 26	26, 48, 115, 133	0
1	E	308/329 (93%)	0.07	15 (4%) 33 22	31, 49, 107, 124	0
1	F	301/329 (91%)	0.35	31 (10%) 9 4	30, 56, 116, 134	0
All	All	1839/1974 (93%)	0.04	82 (4%) 37 26	21, 42, 104, 134	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	LYS	5.6
1	F	260	GLY	5.2
1	B	250	ASN	5.1
1	F	253	PHE	5.0
1	B	248	ALA	4.5
1	F	254	GLU	4.3
1	E	250	ASN	4.3
1	C	248	ALA	4.2
1	F	319	CYS	4.0
1	D	250	ASN	3.8
1	F	310	HIS	3.7
1	F	257	LEU	3.7
1	C	250	ASN	3.7
1	E	245	HIS	3.5
1	F	318	TYR	3.5
1	D	319	CYS	3.4
1	E	323	LEU	3.4
1	F	326	ALA	3.4
1	F	323	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	323	LEU	3.4
1	F	316	ILE	3.4
1	B	245	HIS	3.3
1	D	322	PRO	3.3
1	C	322	PRO	3.3
1	D	245	HIS	3.3
1	F	308	ARG	3.2
1	E	252	THR	3.2
1	F	322	PRO	3.2
1	E	317	THR	3.2
1	B	363	HIS	3.2
1	E	312	PRO	3.2
1	A	250	ASN	3.1
1	F	245	HIS	3.1
1	E	249	LYS	3.1
1	E	313	ASP	3.1
1	F	311	ALA	3.0
1	E	322	PRO	2.8
1	F	314	PHE	2.8
1	D	310	HIS	2.8
1	F	313	ASP	2.8
1	B	251	GLY	2.7
1	F	301	GLU	2.7
1	F	309	LYS	2.7
1	A	245	HIS	2.7
1	D	318	TYR	2.7
1	F	320	VAL	2.7
1	D	363	HIS	2.6
1	D	307	LEU	2.6
1	B	313	ASP	2.6
1	C	313	ASP	2.6
1	B	323	LEU	2.5
1	A	363	HIS	2.5
1	F	261	THR	2.4
1	B	246	ALA	2.4
1	F	284	GLU	2.4
1	D	320	VAL	2.4
1	F	285	ARG	2.4
1	D	257	LEU	2.4
1	F	307	LEU	2.3
1	E	319	CYS	2.3
1	F	255	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	353	PRO	2.3
1	B	318	TYR	2.3
1	E	318	TYR	2.2
1	E	139	ASN	2.2
1	F	360	LEU	2.2
1	F	305	GLN	2.2
1	D	258	GLU	2.2
1	C	363	HIS	2.2
1	F	315	GLN	2.2
1	E	362	PHE	2.1
1	D	313	ASP	2.1
1	D	357	ALA	2.1
1	F	361	ASN	2.1
1	F	230	SER	2.1
1	A	251	GLY	2.1
1	E	255	CYS	2.1
1	D	362	PHE	2.1
1	E	363	HIS	2.0
1	B	247	ALA	2.0
1	F	252	THR	2.0
1	C	320	VAL	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	GOL	A	1002	6/6	0.90	0.37	5.30	42,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	C	1002	6/6	0.89	0.29	3.78	54,55,55,55	0
3	GOL	B	1002	6/6	0.91	0.28	2.55	41,43,44,44	0
2	NAD	F	1001	44/44	0.95	0.20	-0.01	34,45,59,60	0
2	NAD	B	1001	44/44	0.97	0.16	-0.46	28,31,33,33	0
2	NAD	E	1001	44/44	0.96	0.16	-0.53	25,34,40,41	0
2	NAD	A	1001	44/44	0.98	0.16	-0.56	19,22,28,28	0
2	NAD	D	1001	44/44	0.97	0.15	-0.67	26,33,40,41	0
2	NAD	C	1001	44/44	0.97	0.15	-0.70	19,23,33,35	0

6.5 Other polymers (i)

There are no such residues in this entry.