



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 03:00 PM GMT

PDB ID : 4J1T
Title : Crystal structure of Thermus thermophilus transhydrogenase heterotrimeric complex of the Alpha1 subunit dimer with the NADP binding domain (domain III) of the Beta subunit in P2(1)
Authors : Yamaguchi, M.; Leung, J.; Schurig Briccio, L.A.; Gennis, R.B.; Stout, C.D.
Deposited on : 2013-02-02
Resolution : 2.37 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

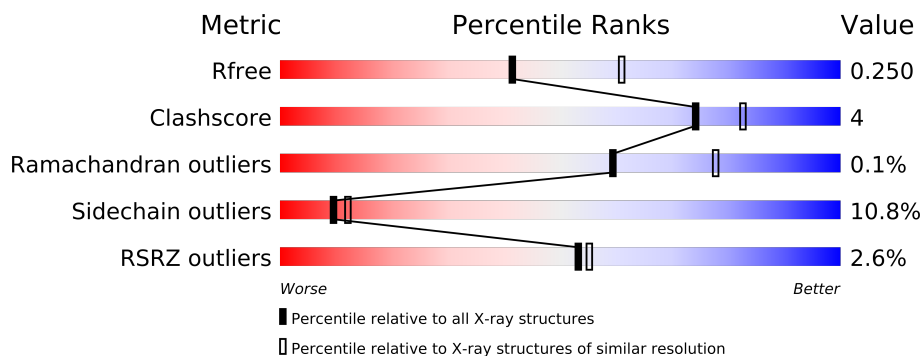
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.37 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}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	381	
1	B	381	
1	D	381	
1	E	381	
2	C	185	
2	F	185	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	A	401	-	X
3	GOL	D	402	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	D	403	-	X
4	NAD	B	500	-	X
4	NAD	E	500	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14253 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NAD/NADP transhydrogenase alpha subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2770	1757	495	506	12			
1	B	367	Total	C	N	O	S	0	0	0
			2765	1755	496	502	12			
1	D	372	Total	C	N	O	S	0	0	0
			2794	1772	498	512	12			
1	E	373	Total	C	N	O	S	0	0	0
			2798	1774	499	513	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-4	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-3	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
A	0	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-5	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-4	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-3	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
B	0	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-5	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-4	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-3	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
D	0	HIS	-	EXPRESSION TAG	UNP Q72GR8
E	-5	HIS	-	EXPRESSION TAG	UNP Q72GR8
E	-4	HIS	-	EXPRESSION TAG	UNP Q72GR8
E	-3	HIS	-	EXPRESSION TAG	UNP Q72GR8

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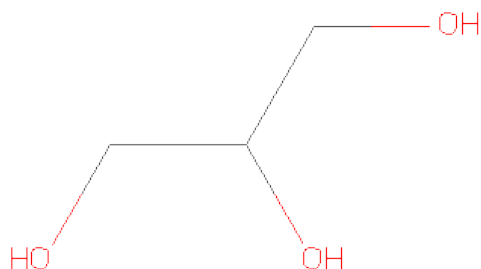
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	EXPRESSION TAG	UNP Q72GR8
E	-1	HIS	-	EXPRESSION TAG	UNP Q72GR8
E	0	HIS	-	EXPRESSION TAG	UNP Q72GR8

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

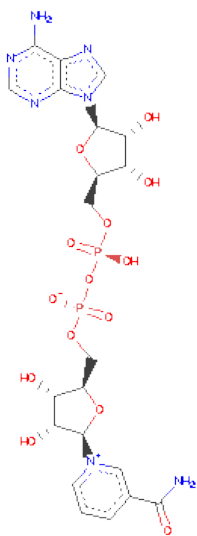
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1343	860	229	248	6			
2	F	177	Total	C	N	O	S	0	0	0
			1343	860	229	248	6			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



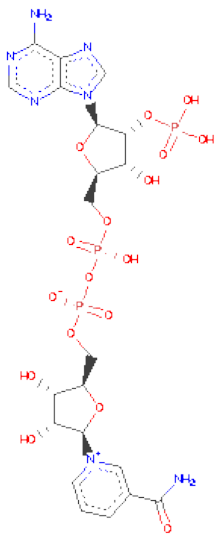
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 6 is water.

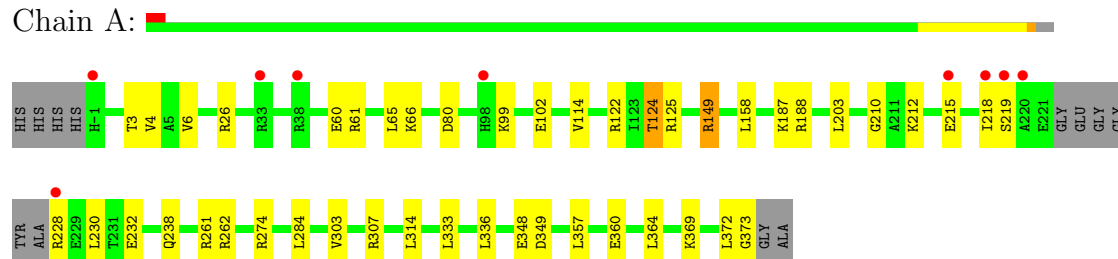
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		
6	B	44	Total	O	0	0
			44	44		
6	C	11	Total	O	0	0
			11	11		
6	D	50	Total	O	0	0
			50	50		
6	E	43	Total	O	0	0
			43	43		
6	F	17	Total	O	0	0
			17	17		

3 Residue-property plots

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.

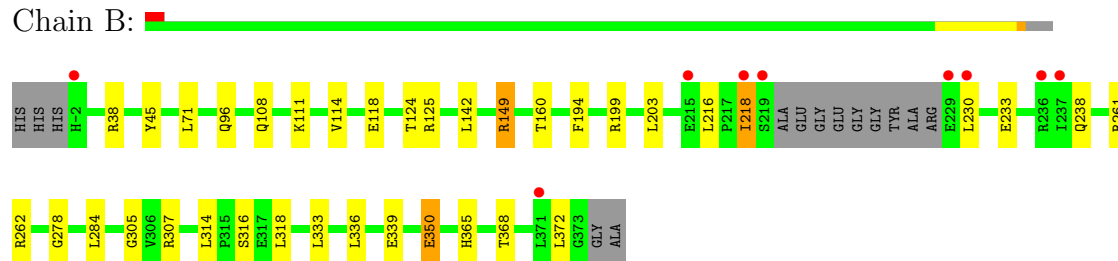
- Molecule 1: NAD/NADP transhydrogenase alpha subunit 1

Chain A:



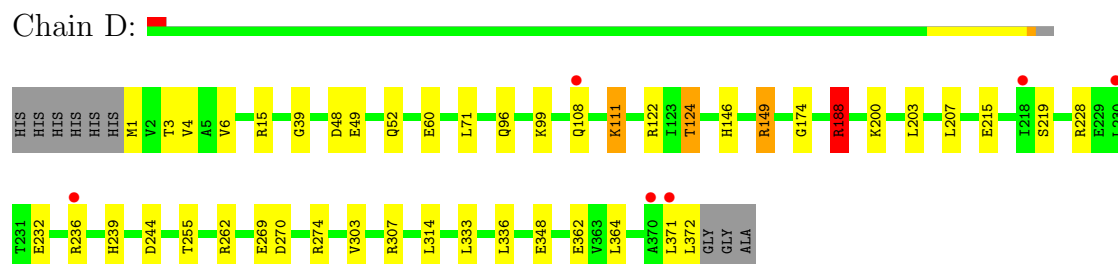
- Molecule 1: NAD/NADP transhydrogenase alpha subunit 1

Chain B:



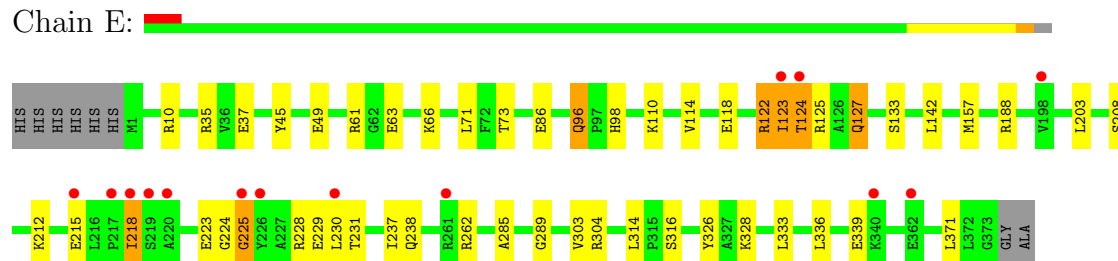
- Molecule 1: NAD/NADP transhydrogenase alpha subunit 1

Chain D:

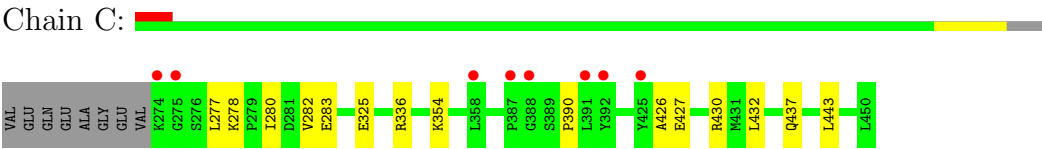


- Molecule 1: NAD/NADP transhydrogenase alpha subunit 1

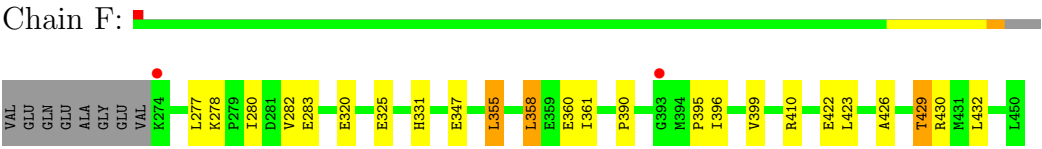
Chain E:



● Molecule 2: NAD(P) transhydrogenase subunit beta



● Molecule 2: NAD(P) transhydrogenase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.08Å 68.87Å 132.34Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	132.35 – 2.37 37.14 – 2.37	Depositor EDS
% Data completeness (in resolution range)	95.2 (132.35-2.37) 95.2 (37.14-2.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.43 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.205 , 0.253 0.201 , 0.250	Depositor DCC
R_{free} test set	4017 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.0	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 79598 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14253	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/2814	0.71	1/3816 (0.0%)
1	B	0.56	0/2812	0.69	0/3814
1	D	0.63	0/2840	0.73	2/3852 (0.1%)
1	E	0.56	0/2844	0.70	1/3857 (0.0%)
2	C	0.51	0/1366	0.64	0/1848
2	F	0.58	0/1366	0.70	1/1848 (0.1%)
All	All	0.58	0/14042	0.70	5/19035 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	E	123	ILE	N-CA-C	-6.00	94.80	111.00
1	A	188	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	188	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	F	358	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2770	0	0	11	0
1	B	2765	0	0	9	0
1	D	2794	0	0	17	0
1	E	2798	0	0	16	0
2	C	1343	0	0	3	0
2	F	1343	0	0	8	0
3	A	6	0	8	4	0
3	D	18	0	24	6	0
4	B	44	0	0	1	0
4	E	44	0	0	1	0
5	C	48	0	0	1	0
5	F	48	0	0	1	0
6	A	67	0	0	1	0
6	B	44	0	0	0	0
6	C	11	0	0	0	0
6	D	50	0	0	1	0
6	E	43	0	0	1	0
6	F	17	0	0	1	0
All	All	14253	0	32	57	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (57) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:146:HIS:ND1	1:D:149:ARG:NH1	1.89	1.19
1:D:188:ARG:CB	3:D:401:GOL:H12	1.89	1.03
1:D:188:ARG:CB	3:D:401:GOL:C1	2.42	0.97
1:D:188:ARG:CB	3:D:401:GOL:H11	2.16	0.74
1:B:365:HIS:ND1	1:B:368:THR:OG1	2.22	0.72
1:A:149:ARG:NE	3:A:401:GOL:H12	2.10	0.67
1:D:111:LYS:NZ	3:D:402:GOL:H31	2.11	0.66
1:D:124:THR:CG2	2:F:390:PRO:O	2.47	0.62
1:E:218:ILE:O	1:E:238:GLN:NE2	2.32	0.61
2:F:410:ARG:NH2	5:F:500:NAP:O1X	2.35	0.58
1:B:199:ARG:NH2	4:B:500:NAD:O3B	2.37	0.57
2:F:278:LYS:NZ	2:F:426:ALA:O	2.38	0.56
1:D:146:HIS:CE1	1:D:149:ARG:NH1	2.71	0.56
1:E:285:ALA:O	1:E:289:GLY:O	2.23	0.56
1:A:307:ARG:NH2	1:B:45:TYR:OH	2.39	0.56
1:A:149:ARG:CG	3:A:401:GOL:O1	2.53	0.56
1:E:157:MET:CE	2:F:355:LEU:CD2	2.84	0.55
1:B:278:GLY:N	1:B:305:GLY:O	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:49:GLU:OE1	1:D:49:GLU:N	2.42	0.53
1:E:122:ARG:NH1	4:E:500:NAD:O2N	2.41	0.53
1:A:125:ARG:NH2	1:A:349:ASP:OD2	2.42	0.53
1:D:111:LYS:NZ	3:D:402:GOL:C3	2.72	0.52
1:D:244:ASP:OD1	1:D:274:ARG:NH1	2.42	0.52
1:A:373:GLY:O	1:D:111:LYS:NZ	2.42	0.52
1:A:149:ARG:NE	3:A:401:GOL:C1	2.73	0.52
1:D:188:ARG:CD	1:E:188:ARG:O	2.58	0.52
3:D:401:GOL:H2	2:F:347:GLU:CA	2.41	0.51
1:D:52:GLN:NE2	6:D:550:HOH:O	2.44	0.51
2:F:331:HIS:NE2	2:F:395:PRO:O	2.44	0.49
1:E:73:THR:O	1:E:326:TYR:OH	2.31	0.48
1:A:274:ARG:NH1	6:A:517:HOH:O	2.45	0.48
1:B:125:ARG:NH1	1:B:350:GLU:OE2	2.47	0.47
1:A:187:LYS:CE	1:A:210:GLY:O	2.63	0.47
1:E:223:GLU:O	1:E:225:GLY:N	2.48	0.47
1:E:35:ARG:NH1	1:E:63:GLU:O	2.48	0.47
1:B:218:ILE:O	1:B:238:GLN:NE2	2.48	0.46
1:E:37:GLU:OE1	1:E:61:ARG:NH1	2.48	0.46
1:E:96:GLN:N	1:E:118:GLU:OE2	2.49	0.46
1:D:174:GLY:O	1:D:255:THR:OG1	2.34	0.46
2:F:422:GLU:CG	6:F:604:HOH:O	2.64	0.46
3:A:401:GOL:H11	1:B:149:ARG:NH2	2.31	0.45
1:E:124:THR:CG2	1:E:127:GLN:OE1	2.65	0.45
1:A:124:THR:CG2	2:C:390:PRO:O	2.65	0.44
1:E:118:GLU:N	1:E:118:GLU:OE1	2.51	0.44
2:C:278:LYS:NZ	2:C:426:ALA:O	2.51	0.44
1:B:96:GLN:N	1:B:118:GLU:OE2	2.51	0.43
1:E:123:ILE:CG1	1:E:123:ILE:O	2.67	0.43
2:F:423:LEU:O	2:F:429:THR:CG2	2.67	0.42
1:E:223:GLU:C	1:E:225:GLY:N	2.73	0.41
1:D:39:GLY:N	1:D:48:ASP:OD1	2.53	0.41
1:B:194:PHE:CD1	1:B:194:PHE:N	2.87	0.41
1:A:61:ARG:NE	1:A:80:ASP:OD2	2.53	0.41
1:D:307:ARG:NH2	1:E:45:TYR:OH	2.54	0.41
1:A:218:ILE:N	1:A:238:GLN:OE1	2.54	0.41
1:E:328:LYS:CD	6:E:620:HOH:O	2.69	0.40
1:D:239:HIS:NE2	1:D:270:ASP:OD2	2.53	0.40
2:C:336:ARG:NH2	5:C:500:NAP:O2A	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/381 (96%)	355 (97%)	10 (3%)	0	100	100
1	B	363/381 (95%)	355 (98%)	8 (2%)	0	100	100
1	D	370/381 (97%)	358 (97%)	12 (3%)	0	100	100
1	E	371/381 (97%)	355 (96%)	14 (4%)	2 (0%)	38	51
2	C	175/185 (95%)	168 (96%)	7 (4%)	0	100	100
2	F	175/185 (95%)	172 (98%)	3 (2%)	0	100	100
All	All	1819/1894 (96%)	1763 (97%)	54 (3%)	2 (0%)	59	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	225	GLY
1	E	224	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/293 (97%)	251 (88%)	34 (12%)	8	9
1	B	286/293 (98%)	260 (91%)	26 (9%)	14	18
1	D	287/293 (98%)	253 (88%)	34 (12%)	8	9
1	E	287/293 (98%)	253 (88%)	34 (12%)	8	9
2	C	139/146 (95%)	128 (92%)	11 (8%)	18	25
2	F	139/146 (95%)	124 (89%)	15 (11%)	9	12
All	All	1423/1464 (97%)	1269 (89%)	154 (11%)	9	12

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	VAL
1	A	6	VAL
1	A	26	ARG
1	A	60	GLU
1	A	65	LEU
1	A	66	LYS
1	A	99	LYS
1	A	102	GLU
1	A	114	VAL
1	A	122	ARG
1	A	124	THR
1	A	149	ARG
1	A	158	LEU
1	A	203	LEU
1	A	212	LYS
1	A	215	GLU
1	A	219	SER
1	A	228	ARG
1	A	230	LEU
1	A	232	GLU
1	A	261	ARG
1	A	262	ARG
1	A	284	LEU
1	A	303	VAL
1	A	314	LEU
1	A	333	LEU
1	A	336	LEU
1	A	348	GLU
1	A	357	LEU
1	A	360	GLU
1	A	364	LEU
1	A	369	LYS
1	A	372	LEU
1	B	38	ARG
1	B	71	LEU
1	B	108	GLN
1	B	111	LYS
1	B	114	VAL
1	B	124	THR
1	B	142	LEU
1	B	149	ARG

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Mol	Chain	Res	Type
1	B	160	THR
1	B	203	LEU
1	B	216	LEU
1	B	218	ILE
1	B	230	LEU
1	B	233	GLU
1	B	261	ARG
1	B	262	ARG
1	B	284	LEU
1	B	307	ARG
1	B	314	LEU
1	B	316	SER
1	B	318	LEU
1	B	333	LEU
1	B	336	LEU
1	B	339	GLU
1	B	350	GLU
1	B	372	LEU
2	C	277	LEU
2	C	280	ILE
2	C	282	VAL
2	C	283	GLU
2	C	325	GLU
2	C	354	LYS
2	C	427	GLU
2	C	430	ARG
2	C	432	LEU
2	C	437	GLN
2	C	443	LEU
1	D	1	MET
1	D	3	THR
1	D	4	VAL
1	D	6	VAL
1	D	15	ARG
1	D	60	GLU
1	D	71	LEU
1	D	96	GLN
1	D	99	LYS
1	D	108	GLN
1	D	111	LYS
1	D	122	ARG
1	D	124	THR

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Mol	Chain	Res	Type
1	D	149	ARG
1	D	188	ARG
1	D	200	LYS
1	D	203	LEU
1	D	207	LEU
1	D	215	GLU
1	D	219	SER
1	D	228	ARG
1	D	232	GLU
1	D	236	ARG
1	D	262	ARG
1	D	269	GLU
1	D	303	VAL
1	D	314	LEU
1	D	333	LEU
1	D	336	LEU
1	D	348	GLU
1	D	362	GLU
1	D	364	LEU
1	D	371	LEU
1	D	372	LEU
1	E	10	ARG
1	E	49	GLU
1	E	66	LYS
1	E	71	LEU
1	E	86	GLU
1	E	96	GLN
1	E	98	HIS
1	E	110	LYS
1	E	114	VAL
1	E	122	ARG
1	E	124	THR
1	E	125	ARG
1	E	127	GLN
1	E	133	SER
1	E	142	LEU
1	E	203	LEU
1	E	208	SER
1	E	212	LYS
1	E	215	GLU
1	E	218	ILE
1	E	228	ARG

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Mol	Chain	Res	Type
1	E	229	GLU
1	E	230	LEU
1	E	231	THR
1	E	237	ILE
1	E	262	ARG
1	E	303	VAL
1	E	304	ARG
1	E	314	LEU
1	E	316	SER
1	E	333	LEU
1	E	336	LEU
1	E	339	GLU
1	E	371	LEU
2	F	277	LEU
2	F	280	ILE
2	F	282	VAL
2	F	283	GLU
2	F	320	GLU
2	F	325	GLU
2	F	355	LEU
2	F	358	LEU
2	F	360	GLU
2	F	361	ILE
2	F	396	ILE
2	F	399	VAL
2	F	429	THR
2	F	430	ARG
2	F	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GOL	A	401	-	5,5,5	0.61	0	5,5,5	1.18	1 (20%)
4	NAD	B	500	-	48,48,48	1.86	9 (18%)	73,73,73	1.89	14 (19%)
5	NAP	C	500	-	52,52,52	1.84	7 (13%)	80,80,80	2.37	20 (25%)
3	GOL	D	401	-	5,5,5	0.50	0	5,5,5	0.91	0
3	GOL	D	402	-	5,5,5	0.44	0	5,5,5	0.79	0
3	GOL	D	403	-	5,5,5	0.34	0	5,5,5	0.67	0
4	NAD	E	500	-	48,48,48	1.87	7 (14%)	73,73,73	2.44	19 (26%)
5	NAP	F	500	-	52,52,52	1.80	9 (17%)	80,80,80	2.42	19 (23%)

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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
4	NAD	B	500	-	-	0/30/62/62	0/3/5/5
5	NAP	C	500	-	-	0/35/67/67	0/3/5/5
3	GOL	D	401	-	-	0/4/4/4	0/0/0/0
3	GOL	D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	D	403	-	-	0/4/4/4	0/0/0/0
4	NAD	E	500	-	-	0/30/62/62	0/3/5/5
5	NAP	F	500	-	-	0/35/67/67	0/3/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	NAD	PN-O2N	7.49	1.66	1.48
4	E	500	NAD	PN-O2N	7.43	1.65	1.48
5	C	500	NAP	PN-O1N	6.74	1.65	1.48
4	B	500	NAD	PN-O1N	6.73	1.65	1.48
4	E	500	NAD	PN-O1N	6.72	1.65	1.48
5	F	500	NAP	PN-O2N	6.63	1.64	1.48
5	F	500	NAP	PN-O1N	6.57	1.64	1.48
5	C	500	NAP	PN-O2N	6.30	1.63	1.48
5	C	500	NAP	P2B-O1X	4.55	1.66	1.51
4	E	500	NAD	PA-O1A	4.12	1.67	1.51
5	C	500	NAP	PA-O1A	4.10	1.67	1.51
4	B	500	NAD	PA-O1A	3.56	1.65	1.51
5	F	500	NAP	P2B-O1X	3.38	1.62	1.51
5	F	500	NAP	PA-O1A	3.13	1.63	1.51
4	B	500	NAD	PA-O3	3.10	1.65	1.59
4	E	500	NAD	PN-O3	2.71	1.65	1.60
5	F	500	NAP	P2B-O2X	2.71	1.64	1.54
4	E	500	NAD	PA-O2A	2.71	1.67	1.55
4	E	500	NAD	PA-O3	2.69	1.64	1.59
5	C	500	NAP	P2B-O2X	2.69	1.64	1.54
5	C	500	NAP	P2B-O3X	2.65	1.64	1.54
5	F	500	NAP	PN-O3	2.55	1.65	1.60
5	F	500	NAP	PA-O3	2.52	1.64	1.59
4	B	500	NAD	PN-O3	2.39	1.65	1.60
4	B	500	NAD	PA-O2A	2.34	1.65	1.55
4	B	500	NAD	O4D-C1D	2.26	1.44	1.41
5	F	500	NAP	P2B-O3X	2.17	1.62	1.54
4	B	500	NAD	PN-O5D	2.14	1.66	1.60
4	B	500	NAD	C4A-N9A	-2.13	1.34	1.37
5	C	500	NAP	PA-O3	2.08	1.63	1.59
5	F	500	NAP	C4N-C3N	2.08	1.42	1.39
4	E	500	NAD	O4D-C1D	2.03	1.44	1.41

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	500	NAP	N3A-C2A-N1A	-12.68	118.11	128.71
5	F	500	NAP	N3A-C2A-N1A	-11.66	118.96	128.71
4	E	500	NAD	O5B-PA-O1A	-9.15	73.53	109.37
4	E	500	NAD	O3-PA-O5B	9.12	144.20	103.41
4	E	500	NAD	N3A-C2A-N1A	-8.28	121.78	128.71
4	B	500	NAD	N3A-C2A-N1A	-7.73	122.24	128.71
5	C	500	NAP	C3N-C7N-N7N	7.57	126.38	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	500	NAP	C3N-C7N-N7N	7.28	126.05	117.77
4	B	500	NAD	C4D-O4D-C1D	-7.24	101.88	109.75
5	F	500	NAP	O4D-C1D-N1N	-5.19	102.64	107.95
5	C	500	NAP	O4B-C1B-C2B	-4.95	102.32	106.95
5	F	500	NAP	O3B-C3B-C4B	-4.94	96.53	111.08
5	F	500	NAP	C4D-O4D-C1D	4.76	114.92	109.75
4	E	500	NAD	O2A-PA-O3	-4.50	83.77	105.14
5	F	500	NAP	O4D-C1D-C2D	-4.48	99.90	106.77
4	E	500	NAD	N3A-C4A-N9A	4.44	133.44	125.43
4	B	500	NAD	O4D-C1D-N1N	4.38	112.43	107.95
4	E	500	NAD	O3-PA-O1A	-4.30	80.45	111.28
4	B	500	NAD	N3A-C4A-N9A	4.22	133.06	125.43
5	F	500	NAP	C6N-N1N-C2N	-4.18	117.32	122.04
5	C	500	NAP	O4B-C1B-N9A	-4.09	104.64	108.44
5	F	500	NAP	N3A-C4A-N9A	4.03	132.72	125.43
4	E	500	NAD	PN-O3-PA	-3.98	115.85	132.95
5	F	500	NAP	O7N-C7N-C3N	-3.97	115.10	119.58
5	C	500	NAP	O7N-C7N-C3N	-3.85	115.23	119.58
5	C	500	NAP	N3A-C4A-N9A	3.66	132.04	125.43
5	C	500	NAP	O3B-C3B-C4B	-3.60	100.46	111.08
5	C	500	NAP	O3D-C3D-C4D	-3.47	100.85	111.08
4	E	500	NAD	O2A-PA-O5B	-3.45	91.12	108.51
4	B	500	NAD	O4D-C4D-C3D	-3.44	98.19	105.17
5	F	500	NAP	O3-PN-O1N	3.20	116.46	108.83
5	C	500	NAP	C8A-N9A-C4A	3.14	109.30	106.90
4	E	500	NAD	C4A-C5A-N7A	-3.10	106.87	109.52
4	B	500	NAD	C4A-C5A-N7A	-3.08	106.88	109.52
5	F	500	NAP	C2A-N3A-C4A	3.07	122.76	114.01
5	C	500	NAP	O7N-C7N-N7N	-2.95	118.33	122.59
4	E	500	NAD	C5A-C4A-N3A	-2.93	119.33	125.70
5	C	500	NAP	O4B-C4B-C3B	-2.92	99.25	105.17
5	C	500	NAP	C4D-O4D-C1D	2.83	112.83	109.75
4	B	500	NAD	C5A-C4A-N3A	-2.83	119.54	125.70
4	E	500	NAD	C5D-C4D-C3D	-2.77	104.13	115.21
5	F	500	NAP	O3D-C3D-C4D	-2.75	102.98	111.08
4	E	500	NAD	O4B-C4B-C5B	-2.74	99.56	109.36
5	C	500	NAP	C2A-N3A-C4A	2.73	121.78	114.01
5	F	500	NAP	C4A-C5A-N7A	-2.73	107.18	109.52
5	F	500	NAP	C5A-C4A-N3A	-2.64	119.95	125.70
5	F	500	NAP	O7N-C7N-N7N	-2.64	118.78	122.59
4	B	500	NAD	O4D-C4D-C5D	2.55	118.48	109.36
5	F	500	NAP	C8A-N9A-C4A	2.54	108.84	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	NAD	O4B-C4B-C5B	-2.48	100.51	109.36
4	E	500	NAD	PA-O5B-C5B	-2.45	104.43	122.03
4	E	500	NAD	C3D-C2D-C1D	2.42	104.69	100.91
5	C	500	NAP	O2N-PN-O3	-2.40	102.33	108.79
5	C	500	NAP	O3X-P2B-O2B	2.33	113.80	107.09
4	B	500	NAD	PN-O3-PA	-2.31	123.01	132.95
4	E	500	NAD	C6N-N1N-C2N	-2.31	119.43	122.04
5	C	500	NAP	C1B-N9A-C4A	-2.27	122.71	126.64
4	E	500	NAD	C8A-N9A-C4A	2.27	108.63	106.90
4	E	500	NAD	C2A-N3A-C4A	2.26	120.45	114.01
4	B	500	NAD	C2D-C3D-C4D	-2.26	98.16	102.65
4	E	500	NAD	O2A-PA-O1A	2.23	124.67	112.21
5	F	500	NAP	O4B-C1B-C2B	-2.20	104.89	106.95
5	F	500	NAP	O2D-C2D-C3D	-2.19	104.70	111.83
4	B	500	NAD	C2A-N3A-C4A	2.14	120.10	114.01
3	A	401	GOL	O2-C2-C1	-2.12	98.56	108.22
5	C	500	NAP	N7A-C8A-N9A	-2.09	108.44	114.36
4	B	500	NAD	C2B-C3B-C4B	2.07	106.78	102.65
5	C	500	NAP	C2A-N1A-C6A	2.06	122.50	118.77
5	C	500	NAP	O4D-C1D-C2D	-2.05	103.64	106.77
5	C	500	NAP	C5A-C4A-N3A	-2.03	121.27	125.70
4	E	500	NAD	C5N-C4N-C3N	-2.03	117.68	120.32
4	B	500	NAD	C5N-C4N-C3N	-2.03	117.68	120.32
5	F	500	NAP	C5N-C6N-N1N	2.02	123.84	120.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	369/381 (96%)	0.24	9 (2%) 56 58	21, 35, 50, 70	0
1	B	367/381 (96%)	0.22	9 (2%) 54 56	21, 40, 59, 70	0
1	D	372/381 (97%)	0.15	6 (1%) 68 71	18, 35, 55, 69	0
1	E	373/381 (97%)	0.39	14 (3%) 38 41	20, 43, 72, 88	0
2	C	177/185 (95%)	0.22	8 (4%) 32 34	25, 44, 60, 70	0
2	F	177/185 (95%)	0.18	2 (1%) 77 80	21, 38, 53, 63	0
All	All	1835/1894 (96%)	0.24	48 (2%) 53 55	18, 38, 59, 88	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	ALA	7.8
1	A	219	SER	5.9
2	F	274	LYS	5.6
1	E	218	ILE	5.4
1	E	217	PRO	4.7
1	A	220	ALA	4.5
1	E	219	SER	4.0
1	B	371	LEU	3.8
1	B	219	SER	3.7
1	E	215	GLU	3.6
1	A	228	ARG	3.6
2	C	275	GLY	3.5
1	D	371	LEU	3.5
1	A	218	ILE	3.3
2	C	387	PRO	3.3
1	B	218	ILE	3.2
1	E	230	LEU	3.2
1	E	124	THR	3.2
1	B	-2	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLU	3.0
1	A	-1	HIS	2.9
2	C	274	LYS	2.8
1	A	98	HIS	2.7
1	B	236	ARG	2.5
1	D	230	LEU	2.5
1	E	123	ILE	2.5
2	C	391	LEU	2.5
2	C	425	TYR	2.5
1	E	362	GLU	2.4
1	A	33	ARG	2.4
1	D	218	ILE	2.4
2	C	388	GLY	2.4
1	D	108	GLN	2.3
1	A	38	ARG	2.3
2	C	392	TYR	2.3
1	E	226	TYR	2.2
1	B	230	LEU	2.2
1	B	237	ILE	2.2
1	D	236	ARG	2.2
1	E	261	ARG	2.1
1	E	340	LYS	2.1
1	D	370	ALA	2.1
2	F	393	GLY	2.1
1	E	198	VAL	2.1
2	C	358	LEU	2.0
1	A	215	GLU	2.0
1	B	215	GLU	2.0
1	E	225	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	D	403	6/6	0.36	8.05	36,38,38,38	0
3	GOL	D	402	6/6	0.35	5.36	33,34,39,41	0
4	NAD	E	500	44/44	0.29	3.94	72,83,102,103	0
4	NAD	B	500	44/44	0.27	3.76	58,71,91,92	0
3	GOL	A	401	6/6	0.24	3.01	30,32,33,37	0
3	GOL	D	401	6/6	0.22	1.70	33,35,35,36	0
5	NAP	F	500	48/48	0.14	-0.31	19,27,32,35	0
5	NAP	C	500	48/48	0.11	-0.60	25,32,36,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.