



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:21 PM GMT

PDB ID : 4E5N
Title : Thermostable phosphite dehydrogenase in complex with NAD
Authors : Zou, Y.; Zhang, H.; Nair, S.K.
Deposited on : 2012-03-14
Resolution : 1.70 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>

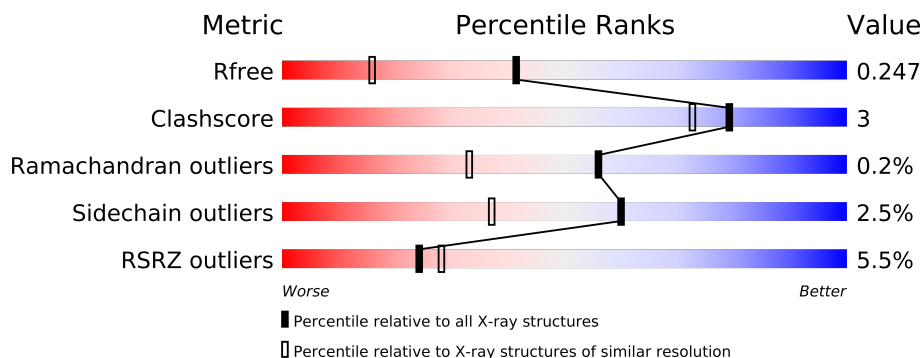
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	330	
1	B	330	
1	C	330	
1	D	330	
1	E	330	
1	F	330	
1	G	330	
1	H	330	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22943 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 Thermostable phosphite dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			
1	B	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			
1	C	330	Total	C	N	O	S	0	0	0
			2528	1597	458	458	15			
1	D	330	Total	C	N	O	S	0	0	0
			2524	1595	457	457	15			
1	E	328	Total	C	N	O	S	0	0	0
			2511	1586	455	456	14			
1	F	327	Total	C	N	O	S	0	0	0
			2504	1581	454	455	14			
1	G	328	Total	C	N	O	S	0	0	0
			2509	1584	455	456	14			
1	H	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	347	Total	O	0	0
			347	347		
3	B	368	Total	O	0	0
			368	368		
3	C	210	Total	O	0	0
			210	210		
3	D	390	Total	O	0	0
			390	390		

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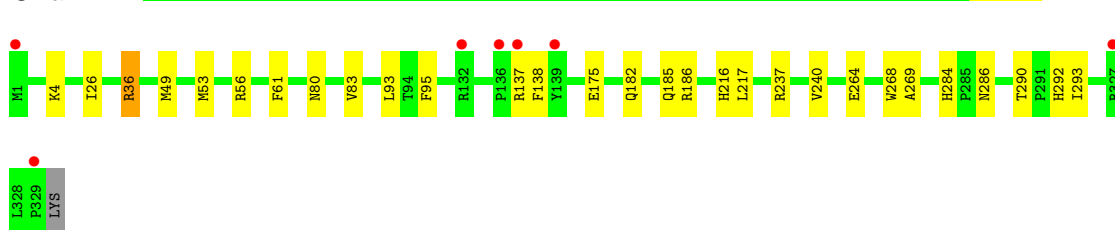
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	235	Total 235	O 235	0	0
3	F	370	Total 370	O 370	0	0
3	G	371	Total 371	O 371	0	0
3	H	167	Total 167	O 167	0	0

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.

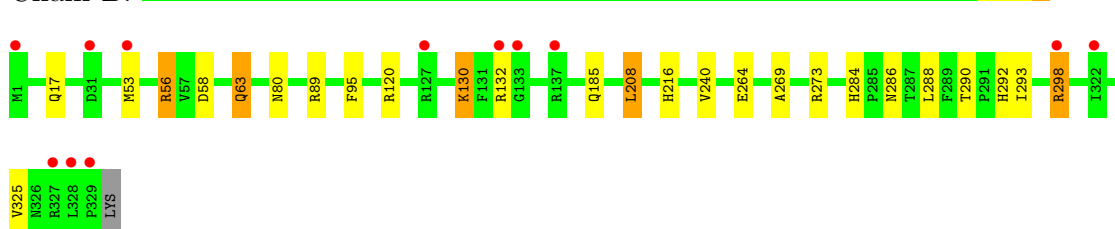
- Molecule 1: Thermostable phosphite dehydrogenase

Chain A:



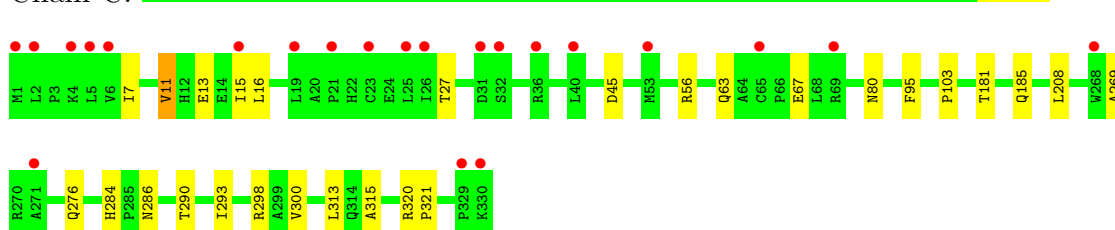
- Molecule 1: Thermostable phosphite dehydrogenase

Chain B:



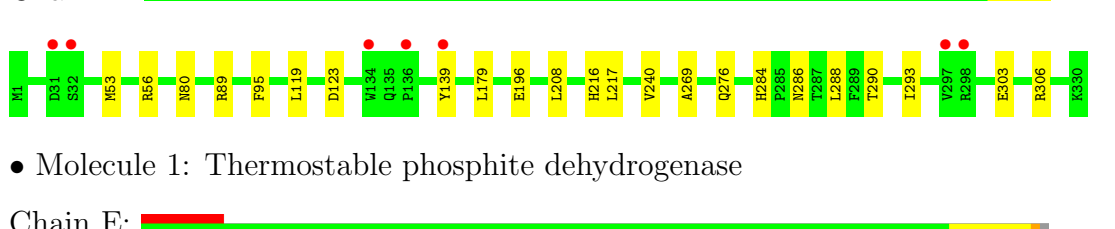
- Molecule 1: Thermostable phosphite dehydrogenase

Chain C:



- Molecule 1: Thermostable phosphite dehydrogenase

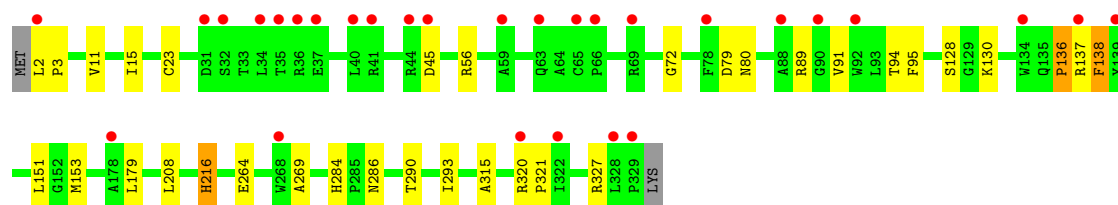
Chain D:



- Molecule 1: Thermostable phosphite dehydrogenase

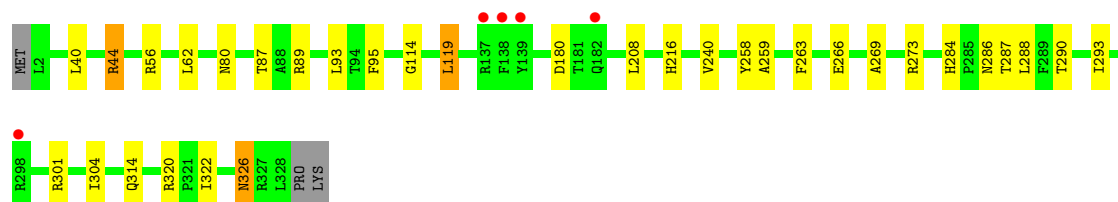
Chain E:





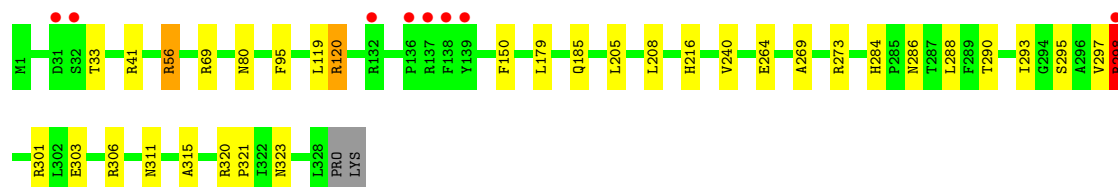
- Molecule 1: Thermostable phosphite dehydrogenase

Chain F:



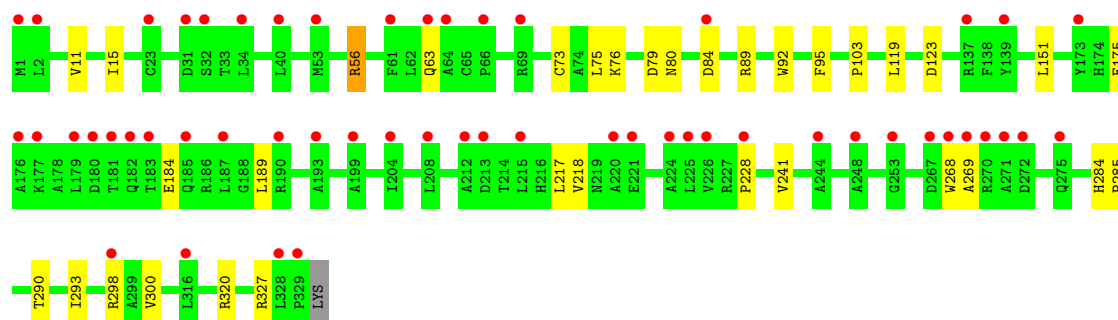
- Molecule 1: Thermostable phosphite dehydrogenase

Chain G:



- Molecule 1: Thermostable phosphite dehydrogenase

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.71Å 113.54Å 130.19Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70 80.19 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-1.70) 95.1 (80.19-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.247 0.211 , 0.247	Depositor DCC
R_{free} test set	13626 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 270433 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22943	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.45 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.3755e-04.*

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: 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	0.38	0/2566	0.56	0/3490
1	B	0.40	0/2566	0.58	0/3490
1	C	0.36	0/2575	0.53	0/3501
1	D	0.41	0/2571	0.57	0/3496
1	E	0.37	0/2558	0.56	0/3480
1	F	0.40	0/2550	0.57	0/3468
1	G	0.41	0/2555	0.57	1/3475 (0.0%)
1	H	0.34	0/2566	0.51	0/3490
All	All	0.38	0/20507	0.56	1/27890 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	120	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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	2519	0	2540	18	0
1	B	2519	0	2540	21	0
1	C	2528	0	2553	13	0
1	D	2524	0	2547	15	0
1	E	2511	0	2528	17	0
1	F	2504	0	2521	24	0
1	G	2509	0	2526	28	0
1	H	2519	0	2540	17	0
2	A	44	0	26	0	0
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	0	0
2	F	44	0	26	0	0
2	G	44	0	26	1	0
2	H	44	0	26	0	0
3	A	347	0	0	0	0
3	B	368	0	0	2	0
3	C	210	0	0	1	0
3	D	390	0	0	5	1
3	E	235	0	0	0	1
3	F	370	0	0	1	1
3	G	371	0	0	4	0
3	H	167	0	0	2	0
All	All	22943	0	20503	143	2

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 3.

All (143) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:56:ARG:NH1	3:G:1263:HOH:O	2.05	0.82
1:G:311:ASN:HD21	1:G:323:ASN:H	1.30	0.79
1:B:298:ARG:O	3:B:1264:HOH:O	2.10	0.70
1:A:290:THR:HB	1:A:293:ILE:HG12	1.77	0.66
1:F:284:HIS:HD2	1:F:286:ASN:H	1.42	0.66
1:D:196:GLU:HG3	3:D:1050:HOH:O	1.96	0.66
1:A:49:MET:HE1	1:A:61:PHE:CE2	2.31	0.66
1:A:284:HIS:HD2	1:A:286:ASN:H	1.42	0.65
1:F:326:ASN:HD22	1:F:326:ASN:H	1.44	0.65
1:A:53:MET:HG2	1:A:292:HIS:CE1	2.32	0.64
1:G:185:GLN:NE2	3:G:997:HOH:O	2.24	0.64
1:E:151:LEU:HG	1:E:208:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:295:SER:OG	1:G:301:ARG:NH1	2.32	0.63
1:D:284:HIS:HD2	1:D:286:ASN:H	1.47	0.62
1:D:139:TYR:CE1	1:G:301:ARG:HG3	2.36	0.61
1:F:44:ARG:HD3	3:F:1005:HOH:O	2.01	0.60
1:A:49:MET:HE1	1:A:61:PHE:HE2	1.67	0.60
1:F:80:ASN:ND2	1:F:269:ALA:H	2.00	0.59
1:G:284:HIS:HD2	1:G:286:ASN:H	1.49	0.59
1:D:303:GLU:OE2	1:D:306:ARG:NH1	2.36	0.59
1:A:284:HIS:CD2	1:A:286:ASN:H	2.19	0.59
1:E:11:VAL:CG1	1:E:15:ILE:HB	2.33	0.59
1:A:36:ARG:NH2	1:A:56:ARG:HH21	2.00	0.58
1:E:216:HIS:HE1	1:E:264:GLU:OE1	1.86	0.58
1:A:4:LYS:HE2	1:A:26:ILE:HG13	1.86	0.58
1:F:208:LEU:HD21	1:F:240:VAL:HG11	1.85	0.57
1:E:315:ALA:HB2	1:E:321:PRO:HG3	1.87	0.57
1:D:196:GLU:OE1	3:D:1275:HOH:O	2.17	0.56
1:B:298:ARG:HD3	1:B:298:ARG:C	2.26	0.56
1:G:303:GLU:OE1	1:G:306:ARG:NH1	2.39	0.55
1:D:119:LEU:HD21	1:G:288:LEU:HD21	1.88	0.55
1:F:114:GLY:HA2	1:F:119:LEU:HD12	1.88	0.55
1:F:314:GLN:HE22	1:F:322:ILE:H	1.52	0.55
1:F:314:GLN:HE22	1:F:322:ILE:HG12	1.70	0.55
1:D:284:HIS:CD2	1:D:286:ASN:H	2.24	0.55
1:C:181:THR:HG22	1:C:185:GLN:HE21	1.71	0.55
1:F:93:LEU:H	1:F:326:ASN:HD21	1.54	0.55
1:B:284:HIS:HD2	1:B:286:ASN:H	1.54	0.55
3:D:980:HOH:O	1:G:298:ARG:HA	2.08	0.54
1:D:139:TYR:HE1	1:G:301:ARG:HG3	1.72	0.54
1:C:298:ARG:HB2	3:C:979:HOH:O	2.07	0.53
1:G:311:ASN:ND2	1:G:323:ASN:H	2.02	0.53
1:B:290:THR:HB	1:B:293:ILE:HG12	1.89	0.53
1:G:80:ASN:ND2	1:G:269:ALA:H	2.07	0.53
1:A:137:ARG:HG2	1:A:138:PHE:H	1.72	0.53
1:F:284:HIS:CD2	1:F:286:ASN:H	2.25	0.52
1:H:290:THR:HB	1:H:293:ILE:HG12	1.91	0.52
1:C:290:THR:HB	1:C:293:ILE:HG12	1.90	0.52
1:D:290:THR:HB	1:D:293:ILE:HG12	1.90	0.52
1:B:208:LEU:HD11	1:B:240:VAL:HG11	1.91	0.52
1:G:208:LEU:HD21	1:G:240:VAL:HG11	1.91	0.52
1:H:320:ARG:HH21	1:H:327:ARG:HG2	1.73	0.52
1:C:284:HIS:HD2	1:C:286:ASN:H	1.57	0.51
1:G:69:ARG:HD2	3:G:1070:HOH:O	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:63:GLN:HE21	1:B:89:ARG:HH12	1.58	0.51
1:D:208:LEU:HD21	1:D:240:VAL:HG11	1.91	0.50
1:F:87:THR:HG22	1:F:326:ASN:HB2	1.93	0.50
1:B:53:MET:HG2	1:B:292:HIS:CE1	2.47	0.50
1:G:303:GLU:OE2	1:G:306:ARG:NH1	2.45	0.49
1:F:62:LEU:HB3	1:F:89:ARG:HD3	1.93	0.49
1:A:36:ARG:HH21	1:A:56:ARG:HH21	1.61	0.48
1:A:80:ASN:ND2	1:A:269:ALA:H	2.11	0.48
1:H:103:PRO:HG3	1:H:300:VAL:HG11	1.94	0.48
1:H:184:GLU:O	1:H:189:LEU:N	2.46	0.48
1:G:216:HIS:HE1	1:G:264:GLU:OE1	1.97	0.48
1:C:11:VAL:HG13	1:C:15:ILE:HB	1.95	0.48
1:G:284:HIS:CD2	1:G:286:ASN:H	2.29	0.48
1:E:89:ARG:HG3	1:E:91:VAL:HG23	1.96	0.48
1:A:216:HIS:HE1	1:A:264:GLU:OE1	1.95	0.48
1:B:216:HIS:HE1	1:B:264:GLU:OE1	1.96	0.48
1:E:284:HIS:CD2	1:E:286:ASN:H	2.32	0.48
1:H:11:VAL:CG1	1:H:15:ILE:HB	2.44	0.47
1:F:314:GLN:NE2	1:F:322:ILE:HG12	2.30	0.47
1:D:80:ASN:ND2	1:D:269:ALA:H	2.13	0.47
1:E:290:THR:HB	1:E:293:ILE:HG12	1.97	0.46
1:C:208:LEU:HD22	2:C:800:NAD:C4A	2.45	0.46
1:A:83:VAL:HG22	1:A:93:LEU:CD2	2.46	0.46
1:G:315:ALA:HB2	1:G:321:PRO:HG3	1.97	0.46
1:E:284:HIS:HD2	1:E:286:ASN:H	1.62	0.46
1:B:120:ARG:HD2	1:H:123:ASP:OD2	2.15	0.46
1:A:182:GLN:O	1:A:186:ARG:HG2	2.16	0.46
1:B:185:GLN:NE2	1:G:273:ARG:HH21	2.15	0.45
1:G:311:ASN:HD21	1:G:323:ASN:N	2.08	0.45
1:C:80:ASN:ND2	1:C:269:ALA:H	2.15	0.45
1:H:218:VAL:HB	1:H:241:VAL:HG12	1.99	0.45
1:B:63:GLN:NE2	1:B:89:ARG:HH12	2.14	0.45
1:H:56:ARG:HG3	1:H:268:TRP:HB2	1.99	0.45
1:E:80:ASN:ND2	1:E:269:ALA:H	2.14	0.45
1:E:136:PRO:O	1:E:138:PHE:N	2.44	0.45
1:B:284:HIS:CD2	1:B:286:ASN:H	2.33	0.44
1:F:263:PHE:O	1:F:266:GLU:HG2	2.17	0.44
2:G:800:NAD:H8A	3:G:1248:HOH:O	2.17	0.44
1:F:93:LEU:H	1:F:326:ASN:ND2	2.15	0.44
1:H:80:ASN:HD22	1:H:269:ALA:HB2	1.82	0.44
1:B:130:LYS:HE2	1:B:132:ARG:HH12	1.82	0.44
1:C:45:ASP:HA	1:C:67:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:151:LEU:HD21	1:H:217:LEU:HD22	2.00	0.44
1:B:208:LEU:CD1	1:B:240:VAL:HG11	2.48	0.43
1:B:288:LEU:HD21	1:H:119:LEU:HD21	2.00	0.43
1:D:89:ARG:HD2	3:D:1007:HOH:O	2.18	0.43
1:B:80:ASN:ND2	1:B:269:ALA:H	2.16	0.43
1:E:128:SER:OG	1:E:130:LYS:HE2	2.18	0.43
1:D:53:MET:HE3	3:D:1274:HOH:O	2.18	0.43
1:E:3:PRO:O	1:E:23:CYS:HB2	2.18	0.43
1:E:72:GLY:HA2	1:E:94:THR:OG1	2.19	0.43
1:G:290:THR:HB	1:G:293:ILE:HG12	2.00	0.43
1:F:301:ARG:HD2	1:F:304:ILE:HD12	2.01	0.43
1:B:63:GLN:HE21	1:B:89:ARG:NH1	2.15	0.43
1:E:153:MET:HG2	1:E:179:LEU:HD11	2.02	0.42
1:G:150:PHE:CE1	1:G:205:LEU:HD12	2.55	0.42
1:B:17:GLN:HG2	3:B:1212:HOH:O	2.19	0.42
1:H:284:HIS:HA	1:H:285:PRO:HD3	1.85	0.42
1:F:314:GLN:NE2	1:F:322:ILE:H	2.17	0.42
1:A:237:ARG:O	1:A:240:VAL:HG22	2.20	0.42
1:F:87:THR:CG2	1:F:326:ASN:HB2	2.49	0.42
1:E:320:ARG:HH21	1:E:327:ARG:NH1	2.17	0.42
1:C:13:GLU:HA	1:C:16:LEU:HD12	2.01	0.42
1:H:89:ARG:NH2	3:H:1031:HOH:O	2.52	0.42
1:C:315:ALA:HB2	1:C:321:PRO:HG3	2.02	0.41
1:B:185:GLN:HE22	1:G:273:ARG:HE	1.67	0.41
1:C:320:ARG:HA	1:C:321:PRO:HD3	1.91	0.41
1:A:36:ARG:NH2	1:A:56:ARG:NH2	2.67	0.41
1:G:303:GLU:CD	1:G:306:ARG:NH1	2.74	0.41
1:B:208:LEU:H	1:B:208:LEU:HD12	1.85	0.41
1:H:73:CYS:HB3	1:H:75:LEU:HG	2.03	0.41
1:A:185:GLN:NE2	1:F:273:ARG:NH1	2.69	0.41
1:F:80:ASN:HD22	1:F:269:ALA:H	1.68	0.41
1:D:288:LEU:HD21	1:G:119:LEU:HD21	2.03	0.41
1:C:103:PRO:HG3	1:C:300:VAL:HG11	2.03	0.41
1:H:92:TRP:CH2	1:H:320:ARG:HG3	2.56	0.41
1:B:56:ARG:CZ	1:B:58:ASP:HB3	2.51	0.41
1:A:36:ARG:HH22	1:A:268:TRP:HB3	1.86	0.41
1:E:2:LEU:HB3	1:E:23:CYS:HA	2.02	0.41
1:E:327:ARG:HD2	1:G:306:ARG:HD3	2.02	0.40
1:F:180:ASP:OD2	1:F:180:ASP:N	2.54	0.40
1:F:258:TYR:O	1:F:287:THR:HA	2.21	0.40
1:F:259:ALA:HA	1:F:288:LEU:O	2.22	0.40
1:D:123:ASP:OD1	1:G:120:ARG:CD	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:290:THR:HB	1:F:293:ILE:HG12	2.03	0.40
1:C:7:ILE:HD12	1:C:27:THR:HG22	2.02	0.40
1:G:297:VAL:CG1	1:G:298:ARG:N	2.84	0.40
1:H:320:ARG:NH2	1:H:327:ARG:HG2	2.36	0.40
1:H:320:ARG:NH1	3:H:1043:HOH:O	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:997:HOH:O	3:F:1270:HOH:O[2_645]	2.13	0.07
3:D:1230:HOH:O	3:E:987:HOH:O[1_545]	2.15	0.05

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	327/330 (99%)	319 (98%)	8 (2%)	0	100	100
1	B	327/330 (99%)	318 (97%)	9 (3%)	0	100	100
1	C	328/330 (99%)	317 (97%)	11 (3%)	0	100	100
1	D	328/330 (99%)	321 (98%)	7 (2%)	0	100	100
1	E	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	33	13
1	F	325/330 (98%)	318 (98%)	7 (2%)	0	100	100
1	G	326/330 (99%)	315 (97%)	9 (3%)	2 (1%)	33	13
1	H	327/330 (99%)	315 (96%)	11 (3%)	1 (0%)	50	27
All	All	2614/2640 (99%)	2536 (97%)	73 (3%)	5 (0%)	56	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	298	ARG
1	E	137	ARG

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Mol	Chain	Res	Type
1	G	33	THR
1	E	136	PRO
1	H	228	PRO

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	259/260 (100%)	255 (98%)	4 (2%)	76	60
1	B	259/260 (100%)	251 (97%)	8 (3%)	52	27
1	C	260/260 (100%)	254 (98%)	6 (2%)	63	41
1	D	259/260 (100%)	253 (98%)	6 (2%)	63	41
1	E	258/260 (99%)	252 (98%)	6 (2%)	63	41
1	F	257/260 (99%)	249 (97%)	8 (3%)	52	27
1	G	257/260 (99%)	251 (98%)	6 (2%)	63	41
1	H	259/260 (100%)	251 (97%)	8 (3%)	52	27
All	All	2068/2080 (99%)	2016 (98%)	52 (2%)	60	37

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	95	PHE
1	A	175	GLU
1	A	217	LEU
1	B	56	ARG
1	B	63	GLN
1	B	95	PHE
1	B	130	LYS
1	B	208	LEU
1	B	273	ARG
1	B	298	ARG
1	B	325	VAL
1	C	11	VAL
1	C	56	ARG

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Mol	Chain	Res	Type
1	C	63	GLN
1	C	95	PHE
1	C	276	GLN
1	C	313	LEU
1	D	56	ARG
1	D	95	PHE
1	D	179	LEU
1	D	216	HIS
1	D	217	LEU
1	D	276	GLN
1	E	45	ASP
1	E	56	ARG
1	E	79	ASP
1	E	95	PHE
1	E	138	PHE
1	E	216	HIS
1	F	40	LEU
1	F	44	ARG
1	F	56	ARG
1	F	95	PHE
1	F	119	LEU
1	F	216	HIS
1	F	320	ARG
1	F	326	ASN
1	G	41	ARG
1	G	56	ARG
1	G	95	PHE
1	G	179	LEU
1	G	298	ARG
1	G	320	ARG
1	H	56	ARG
1	H	63	GLN
1	H	76	LYS
1	H	79	ASP
1	H	84	ASP
1	H	95	PHE
1	H	175	GLU
1	H	298	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	80	ASN
1	A	135	GLN
1	A	165	GLN
1	A	185	GLN
1	A	216	HIS
1	A	276	GLN
1	A	284	HIS
1	B	28	ASN
1	B	63	GLN
1	B	80	ASN
1	B	165	GLN
1	B	182	GLN
1	B	185	GLN
1	B	216	HIS
1	B	276	GLN
1	B	284	HIS
1	C	28	ASN
1	C	63	GLN
1	C	80	ASN
1	C	165	GLN
1	C	185	GLN
1	C	216	HIS
1	C	276	GLN
1	C	284	HIS
1	D	28	ASN
1	D	80	ASN
1	D	165	GLN
1	D	216	HIS
1	D	275	GLN
1	D	284	HIS
1	E	17	GLN
1	E	28	ASN
1	E	80	ASN
1	E	216	HIS
1	E	284	HIS
1	F	9	HIS
1	F	80	ASN
1	F	165	GLN
1	F	185	GLN
1	F	216	HIS
1	F	276	GLN
1	F	284	HIS

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Mol	Chain	Res	Type
1	F	314	GLN
1	F	326	ASN
1	G	80	ASN
1	G	165	GLN
1	G	216	HIS
1	G	284	HIS
1	G	311	ASN
1	H	28	ASN
1	H	80	ASN
1	H	118	HIS

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$
2	NAD	A	800	-	48,48,48	0.77	2 (4%)	73,73,73	1.71	11 (15%)
2	NAD	B	800	-	48,48,48	0.79	2 (4%)	73,73,73	1.78	10 (13%)
2	NAD	C	800	-	48,48,48	0.76	1 (2%)	73,73,73	1.76	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	800	-	48,48,48	0.68	1 (2%)	73,73,73	1.63	10 (13%)
2	NAD	E	800	-	48,48,48	0.79	1 (2%)	73,73,73	1.66	11 (15%)
2	NAD	F	800	-	48,48,48	0.77	1 (2%)	73,73,73	1.66	11 (15%)
2	NAD	G	800	-	48,48,48	0.80	1 (2%)	73,73,73	1.74	8 (10%)
2	NAD	H	800	-	48,48,48	0.76	1 (2%)	73,73,73	1.66	10 (13%)

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	800	-	-	0/30/62/62	0/3/5/5
2	NAD	B	800	-	-	0/30/62/62	0/3/5/5
2	NAD	C	800	-	-	0/30/62/62	0/3/5/5
2	NAD	D	800	-	-	0/30/62/62	0/3/5/5
2	NAD	E	800	-	-	0/30/62/62	0/3/5/5
2	NAD	F	800	-	-	0/30/62/62	0/3/5/5
2	NAD	G	800	-	-	0/30/62/62	0/3/5/5
2	NAD	H	800	-	-	0/30/62/62	0/3/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	NAD	C4A-N9A	-2.91	1.33	1.37
2	G	800	NAD	C4A-N9A	-2.88	1.33	1.37
2	A	800	NAD	C4A-N9A	-2.87	1.33	1.37
2	C	800	NAD	C4A-N9A	-2.62	1.33	1.37
2	F	800	NAD	C4A-N9A	-2.55	1.34	1.37
2	E	800	NAD	C4A-N9A	-2.42	1.34	1.37
2	H	800	NAD	C4A-N9A	-2.41	1.34	1.37
2	D	800	NAD	C4A-N9A	-2.39	1.34	1.37
2	B	800	NAD	O4D-C1D	2.03	1.44	1.41
2	A	800	NAD	O4D-C1D	2.02	1.44	1.41

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	NAD	N3A-C2A-N1A	-9.79	120.52	128.71
2	B	800	NAD	N3A-C2A-N1A	-9.70	120.60	128.71
2	G	800	NAD	N3A-C2A-N1A	-9.66	120.63	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	NAD	N3A-C2A-N1A	-9.63	120.66	128.71
2	E	800	NAD	N3A-C2A-N1A	-9.46	120.80	128.71
2	F	800	NAD	N3A-C2A-N1A	-9.37	120.88	128.71
2	C	800	NAD	N3A-C2A-N1A	-9.26	120.97	128.71
2	H	800	NAD	N3A-C2A-N1A	-9.13	121.07	128.71
2	C	800	NAD	O4B-C1B-N9A	6.41	114.40	108.44
2	B	800	NAD	O4B-C1B-N9A	5.70	113.75	108.44
2	G	800	NAD	O4B-C1B-N9A	5.37	113.43	108.44
2	A	800	NAD	O4B-C1B-N9A	5.34	113.41	108.44
2	H	800	NAD	O4B-C1B-N9A	5.23	113.31	108.44
2	F	800	NAD	O4B-C1B-N9A	4.20	112.35	108.44
2	C	800	NAD	N3A-C4A-N9A	4.08	132.81	125.43
2	H	800	NAD	N3A-C4A-N9A	4.08	132.80	125.43
2	E	800	NAD	N3A-C4A-N9A	4.01	132.68	125.43
2	F	800	NAD	N3A-C4A-N9A	3.89	132.46	125.43
2	G	800	NAD	N3A-C4A-N9A	3.84	132.37	125.43
2	B	800	NAD	N3A-C4A-N9A	3.81	132.31	125.43
2	D	800	NAD	N3A-C4A-N9A	3.77	132.24	125.43
2	A	800	NAD	N3A-C4A-N9A	3.76	132.23	125.43
2	E	800	NAD	O4B-C1B-N9A	3.67	111.85	108.44
2	B	800	NAD	C4B-O4B-C1B	-3.60	105.84	109.75
2	C	800	NAD	O4D-C1D-N1N	3.47	111.50	107.95
2	G	800	NAD	C4B-O4B-C1B	-3.17	106.31	109.75
2	H	800	NAD	O4D-C1D-N1N	3.16	111.18	107.95
2	B	800	NAD	C8A-N9A-C4A	3.15	109.30	106.90
2	D	800	NAD	C4A-C5A-N7A	-3.12	106.85	109.52
2	F	800	NAD	C4B-O4B-C1B	-3.01	106.48	109.75
2	E	800	NAD	O4D-C1D-N1N	2.90	110.92	107.95
2	C	800	NAD	C5A-C4A-N3A	-2.80	119.59	125.70
2	H	800	NAD	C5A-C4A-N3A	-2.77	119.67	125.70
2	D	800	NAD	C5A-C4A-N3A	-2.72	119.78	125.70
2	C	800	NAD	C3D-C2D-C1D	2.71	105.14	100.91
2	A	800	NAD	C4B-O4B-C1B	-2.69	106.82	109.75
2	E	800	NAD	C5A-C4A-N3A	-2.69	119.85	125.70
2	F	800	NAD	C5A-C4A-N3A	-2.67	119.89	125.70
2	G	800	NAD	C5A-C4A-N3A	-2.64	119.96	125.70
2	D	800	NAD	O4B-C1B-N9A	2.63	110.89	108.44
2	H	800	NAD	C3D-C2D-C1D	2.62	105.02	100.91
2	E	800	NAD	C3N-C7N-N7N	2.62	120.76	117.77
2	B	800	NAD	C1B-N9A-C4A	-2.57	122.19	126.64
2	A	800	NAD	C5A-C4A-N3A	-2.56	120.12	125.70
2	B	800	NAD	C4A-C5A-N7A	-2.53	107.36	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	NAD	C5A-C4A-N3A	-2.50	120.25	125.70
2	D	800	NAD	C2A-N3A-C4A	2.48	121.06	114.01
2	E	800	NAD	C4A-C5A-N7A	-2.42	107.44	109.52
2	C	800	NAD	C4A-C5A-N7A	-2.42	107.44	109.52
2	G	800	NAD	C4A-C5A-N7A	-2.42	107.45	109.52
2	F	800	NAD	C4A-C5A-N7A	-2.40	107.47	109.52
2	D	800	NAD	C4B-O4B-C1B	-2.38	107.16	109.75
2	D	800	NAD	C1B-N9A-C4A	-2.37	122.54	126.64
2	H	800	NAD	C4A-C5A-N7A	-2.35	107.50	109.52
2	E	800	NAD	C8A-N9A-C4A	2.31	108.67	106.90
2	F	800	NAD	C3D-C2D-C1D	2.28	104.47	100.91
2	B	800	NAD	C2A-N3A-C4A	2.27	120.48	114.01
2	A	800	NAD	C8A-N9A-C4A	2.27	108.63	106.90
2	D	800	NAD	C8A-N9A-C4A	2.27	108.63	106.90
2	G	800	NAD	C2A-N3A-C4A	2.27	120.47	114.01
2	F	800	NAD	C2A-N3A-C4A	2.25	120.41	114.01
2	F	800	NAD	C8A-N9A-C4A	2.25	108.61	106.90
2	E	800	NAD	C2A-N3A-C4A	2.24	120.39	114.01
2	H	800	NAD	C2A-N3A-C4A	2.23	120.37	114.01
2	A	800	NAD	C2A-N3A-C4A	2.23	120.36	114.01
2	B	800	NAD	N7A-C8A-N9A	-2.23	108.05	114.36
2	C	800	NAD	C2A-N3A-C4A	2.20	120.27	114.01
2	A	800	NAD	C4A-C5A-N7A	-2.16	107.67	109.52
2	D	800	NAD	N7A-C8A-N9A	-2.15	108.28	114.36
2	A	800	NAD	C3D-C2D-C1D	2.13	104.24	100.91
2	E	800	NAD	C4B-O4B-C1B	-2.12	107.45	109.75
2	H	800	NAD	C8A-N9A-C4A	2.10	108.50	106.90
2	F	800	NAD	O4D-C1D-N1N	2.06	110.05	107.95
2	H	800	NAD	PN-O3-PA	-2.05	124.13	132.95
2	A	800	NAD	C1B-N9A-C4A	-2.05	123.09	126.64
2	F	800	NAD	N7A-C8A-N9A	-2.03	108.61	114.36
2	E	800	NAD	N7A-C8A-N9A	-2.03	108.62	114.36
2	A	800	NAD	N7A-C8A-N9A	-2.03	108.62	114.36
2	G	800	NAD	C8A-N9A-C4A	2.02	108.44	106.90

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	329/330 (99%)	0.13	7 (2%) 60 66	17, 24, 37, 47	0
1	B	329/330 (99%)	0.17	12 (3%) 41 46	15, 23, 39, 52	0
1	C	330/330 (100%)	0.44	22 (6%) 17 21	19, 31, 55, 61	0
1	D	330/330 (100%)	-0.01	7 (2%) 60 66	14, 21, 36, 45	0
1	E	328/330 (99%)	0.48	29 (8%) 10 13	17, 29, 53, 64	0
1	F	327/330 (99%)	0.03	5 (1%) 70 76	16, 24, 37, 46	0
1	G	328/330 (99%)	0.11	8 (2%) 56 61	14, 22, 38, 43	0
1	H	329/330 (99%)	1.05	54 (16%) 2 3	24, 40, 60, 65	0
All	All	2630/2640 (99%)	0.30	144 (5%) 24 28	14, 26, 50, 65	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	6.2
1	H	271	ALA	5.6
1	G	31	ASP	5.4
1	H	1	MET	5.4
1	E	137	ARG	5.0
1	B	1	MET	5.0
1	G	32	SER	4.9
1	C	271	ALA	4.9
1	E	88	ALA	4.9
1	E	63	GLN	4.7
1	D	134	TRP	4.4
1	H	225	LEU	4.3
1	A	139	TYR	4.2
1	B	329	PRO	4.1
1	A	136	PRO	4.1
1	E	139	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	328	LEU	4.0
1	G	136	PRO	4.0
1	H	268	TRP	4.0
1	B	298	ARG	4.0
1	A	1	MET	4.0
1	H	329	PRO	3.9
1	H	269	ALA	3.9
1	E	44	ARG	3.8
1	H	316	LEU	3.7
1	H	253	GLY	3.7
1	E	35	THR	3.6
1	H	183	THR	3.6
1	H	179	LEU	3.6
1	B	327	ARG	3.6
1	C	26	ILE	3.5
1	H	328	LEU	3.5
1	E	34	LEU	3.5
1	C	36	ARG	3.4
1	D	32	SER	3.4
1	H	181	THR	3.4
1	H	193	ALA	3.3
1	B	133	GLY	3.3
1	E	31	ASP	3.3
1	B	127	ARG	3.3
1	H	176	ALA	3.2
1	E	329	PRO	3.2
1	A	329	PRO	3.2
1	G	138	PHE	3.1
1	H	228	PRO	3.1
1	D	298	ARG	3.1
1	C	5	LEU	3.0
1	H	69	ARG	3.0
1	H	23	CYS	3.0
1	A	137	ARG	2.9
1	D	136	PRO	2.9
1	C	4	LYS	2.9
1	E	32	SER	2.8
1	E	328	LEU	2.8
1	E	36	ARG	2.8
1	C	69	ARG	2.7
1	C	21	PRO	2.7
1	F	138	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	320	ARG	2.7
1	H	221	GLU	2.7
1	C	330	LYS	2.7
1	H	208	LEU	2.7
1	E	37	GLU	2.7
1	F	137	ARG	2.7
1	E	45	ASP	2.7
1	F	298	ARG	2.7
1	E	41	ARG	2.7
1	C	329	PRO	2.7
1	D	31	ASP	2.7
1	H	53	MET	2.7
1	A	327	ARG	2.7
1	C	2	LEU	2.6
1	A	132	ARG	2.6
1	H	224	ALA	2.6
1	C	65	CYS	2.6
1	B	137	ARG	2.6
1	E	40	LEU	2.6
1	E	69	ARG	2.6
1	E	178	ALA	2.6
1	C	15	ILE	2.6
1	D	139	TYR	2.5
1	H	2	LEU	2.5
1	H	139	TYR	2.5
1	H	187	LEU	2.5
1	C	23	CYS	2.5
1	C	19	LEU	2.5
1	G	298	ARG	2.5
1	B	31	ASP	2.5
1	F	182	GLN	2.5
1	H	63	GLN	2.5
1	B	132	ARG	2.4
1	H	40	LEU	2.4
1	F	139	TYR	2.4
1	E	134	TRP	2.4
1	H	185	GLN	2.4
1	H	212	ALA	2.4
1	H	220	ALA	2.4
1	H	31	ASP	2.3
1	E	322	ILE	2.3
1	H	182	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	137	ARG	2.3
1	H	248	ALA	2.3
1	H	177	LYS	2.3
1	C	268	TRP	2.3
1	H	272	ASP	2.3
1	E	78	PHE	2.3
1	H	215	LEU	2.3
1	G	132	ARG	2.3
1	H	32	SER	2.3
1	H	190	ARG	2.3
1	H	64	ALA	2.3
1	H	267	ASP	2.3
1	C	25	LEU	2.2
1	H	34	LEU	2.2
1	E	65	CYS	2.2
1	H	270	ARG	2.2
1	H	173	TYR	2.2
1	C	32	SER	2.2
1	E	268	TRP	2.2
1	G	139	TYR	2.2
1	H	204	ILE	2.2
1	H	199	ALA	2.2
1	H	244	ALA	2.2
1	C	31	ASP	2.1
1	H	180	ASP	2.1
1	E	2	LEU	2.1
1	G	137	ARG	2.1
1	B	53	MET	2.1
1	E	59	ALA	2.1
1	C	53	MET	2.1
1	H	213	ASP	2.1
1	H	298	ARG	2.1
1	C	40	LEU	2.1
1	E	90	GLY	2.0
1	C	6	VAL	2.0
1	B	322	ILE	2.0
1	H	61	PHE	2.0
1	E	66	PRO	2.0
1	H	66	PRO	2.0
1	D	297	VAL	2.0
1	H	84	ASP	2.0
1	H	226	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	92	TRP	2.0
1	H	275	GLN	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
2	NAD	F	800	44/44	0.08	-0.20	18,19,23,24	0
2	NAD	D	800	44/44	0.08	-0.22	16,18,22,23	0
2	NAD	C	800	44/44	0.09	-0.24	21,24,33,34	0
2	NAD	H	800	44/44	0.12	-0.40	35,38,47,47	0
2	NAD	G	800	44/44	0.08	-0.54	15,18,21,22	0
2	NAD	A	800	44/44	0.08	-0.73	18,22,25,25	0
2	NAD	B	800	44/44	0.08	-0.88	13,16,18,21	0
2	NAD	E	800	44/44	0.07	-1.23	21,24,27,29	0

6.5 Other polymers

There are no such residues in this entry.