



Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2017 – 12:12 PM EDT

PDB ID : 5VMT
Title : Crystal structure of a glyceraldehyde-3-phosphate dehydrogenase from
Neisseria gonorrhoeae bound to NAD
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2017-04-28
Resolution : 2.50 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029077

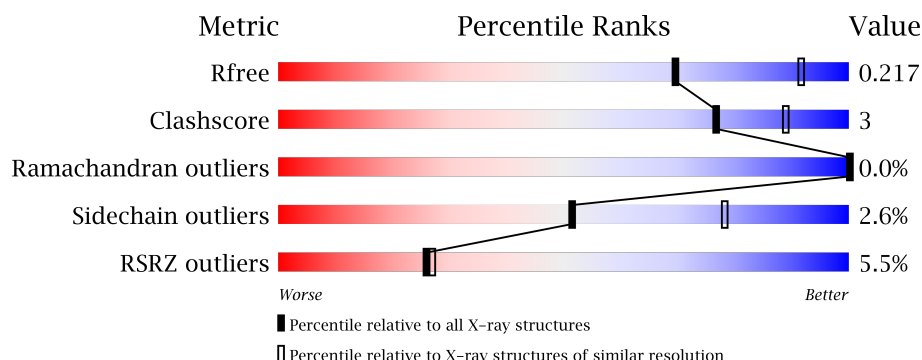
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 $\leq 5\%$. 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	342	<div> <div>0.0%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>0.0%</div> </div> </div>
1	B	342	<div> <div></div> <div> <div>89%</div> <div>7%</div> <div>0.0%</div> </div> </div>
1	C	342	<div> <div>12%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	D	342	<div> <div></div> <div> <div>88%</div> <div>10%</div> <div>0.0%</div> </div> </div>
1	E	342	<div> <div>13%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	342	 <p>2% 90% 6%</p>
1	G	342	 <p>10% 91% 6%</p>
1	H	342	 <p>4% 86% 11%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20034 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2477	1552	429	486	10			
1	B	334	Total	C	N	O	S	0	0	0
			2480	1555	431	484	10			
1	C	325	Total	C	N	O	S	0	0	0
			2308	1441	404	453	10			
1	D	334	Total	C	N	O	S	0	0	0
			2475	1552	431	481	11			
1	E	293	Total	C	N	O	S	0	0	0
			2073	1287	359	417	10			
1	F	333	Total	C	N	O	S	0	2	0
			2484	1557	431	486	10			
1	G	332	Total	C	N	O	S	0	0	0
			2352	1466	407	469	10			
1	H	332	Total	C	N	O	S	0	0	0
			2381	1490	411	470	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP B4RPP8
A	-6	ALA	-	expression tag	UNP B4RPP8
A	-5	HIS	-	expression tag	UNP B4RPP8
A	-4	HIS	-	expression tag	UNP B4RPP8
A	-3	HIS	-	expression tag	UNP B4RPP8
A	-2	HIS	-	expression tag	UNP B4RPP8
A	-1	HIS	-	expression tag	UNP B4RPP8
A	0	HIS	-	expression tag	UNP B4RPP8
B	-7	MET	-	initiating methionine	UNP B4RPP8
B	-6	ALA	-	expression tag	UNP B4RPP8
B	-5	HIS	-	expression tag	UNP B4RPP8
B	-4	HIS	-	expression tag	UNP B4RPP8
B	-3	HIS	-	expression tag	UNP B4RPP8

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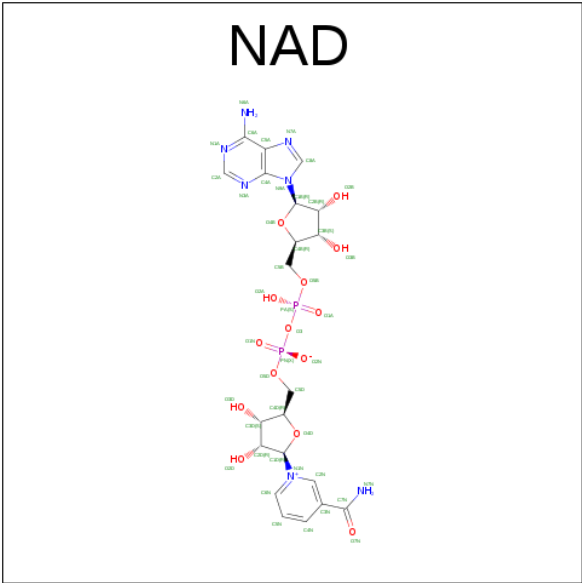
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B4RPP8
B	-1	HIS	-	expression tag	UNP B4RPP8
B	0	HIS	-	expression tag	UNP B4RPP8
C	-7	MET	-	initiating methionine	UNP B4RPP8
C	-6	ALA	-	expression tag	UNP B4RPP8
C	-5	HIS	-	expression tag	UNP B4RPP8
C	-4	HIS	-	expression tag	UNP B4RPP8
C	-3	HIS	-	expression tag	UNP B4RPP8
C	-2	HIS	-	expression tag	UNP B4RPP8
C	-1	HIS	-	expression tag	UNP B4RPP8
C	0	HIS	-	expression tag	UNP B4RPP8
D	-7	MET	-	initiating methionine	UNP B4RPP8
D	-6	ALA	-	expression tag	UNP B4RPP8
D	-5	HIS	-	expression tag	UNP B4RPP8
D	-4	HIS	-	expression tag	UNP B4RPP8
D	-3	HIS	-	expression tag	UNP B4RPP8
D	-2	HIS	-	expression tag	UNP B4RPP8
D	-1	HIS	-	expression tag	UNP B4RPP8
D	0	HIS	-	expression tag	UNP B4RPP8
E	-7	MET	-	initiating methionine	UNP B4RPP8
E	-6	ALA	-	expression tag	UNP B4RPP8
E	-5	HIS	-	expression tag	UNP B4RPP8
E	-4	HIS	-	expression tag	UNP B4RPP8
E	-3	HIS	-	expression tag	UNP B4RPP8
E	-2	HIS	-	expression tag	UNP B4RPP8
E	-1	HIS	-	expression tag	UNP B4RPP8
E	0	HIS	-	expression tag	UNP B4RPP8
F	-7	MET	-	initiating methionine	UNP B4RPP8
F	-6	ALA	-	expression tag	UNP B4RPP8
F	-5	HIS	-	expression tag	UNP B4RPP8
F	-4	HIS	-	expression tag	UNP B4RPP8
F	-3	HIS	-	expression tag	UNP B4RPP8
F	-2	HIS	-	expression tag	UNP B4RPP8
F	-1	HIS	-	expression tag	UNP B4RPP8
F	0	HIS	-	expression tag	UNP B4RPP8
G	-7	MET	-	initiating methionine	UNP B4RPP8
G	-6	ALA	-	expression tag	UNP B4RPP8
G	-5	HIS	-	expression tag	UNP B4RPP8
G	-4	HIS	-	expression tag	UNP B4RPP8
G	-3	HIS	-	expression tag	UNP B4RPP8
G	-2	HIS	-	expression tag	UNP B4RPP8
G	-1	HIS	-	expression tag	UNP B4RPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP B4RPP8
H	-7	MET	-	initiating methionine	UNP B4RPP8
H	-6	ALA	-	expression tag	UNP B4RPP8
H	-5	HIS	-	expression tag	UNP B4RPP8
H	-4	HIS	-	expression tag	UNP B4RPP8
H	-3	HIS	-	expression tag	UNP B4RPP8
H	-2	HIS	-	expression tag	UNP B4RPP8
H	-1	HIS	-	expression tag	UNP B4RPP8
H	0	HIS	-	expression tag	UNP B4RPP8

- 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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

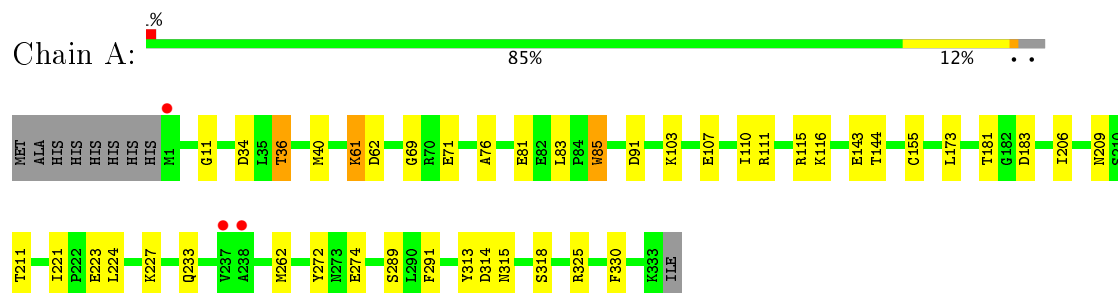
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		
4	B	129	Total	O	0	0
			129	129		
4	C	60	Total	O	0	0
			60	60		
4	D	113	Total	O	0	0
			113	113		
4	E	52	Total	O	0	0
			52	52		
4	F	118	Total	O	0	0
			118	118		
4	G	21	Total	O	0	0
			21	21		
4	H	42	Total	O	0	0
			42	42		

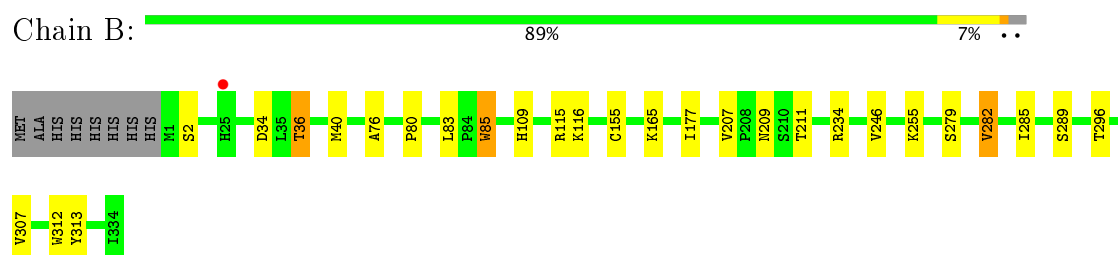
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

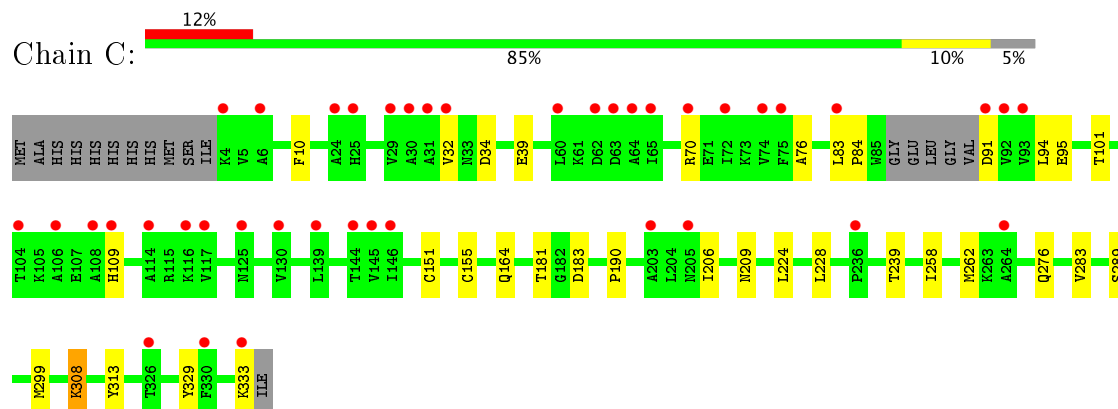
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

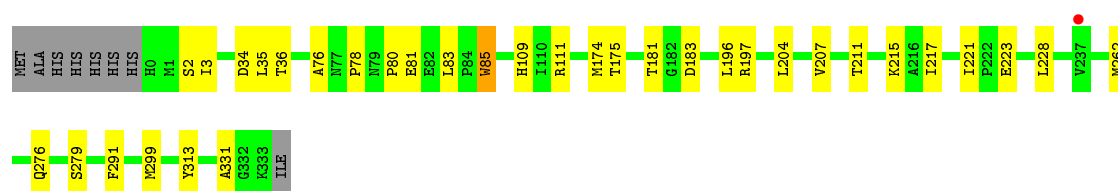


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

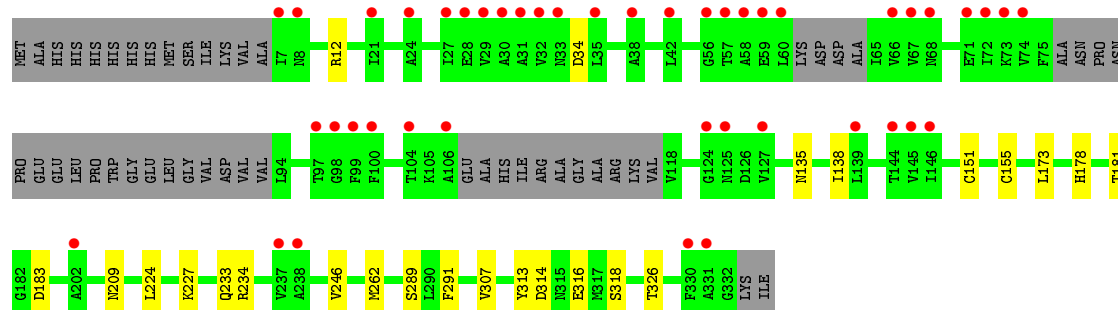
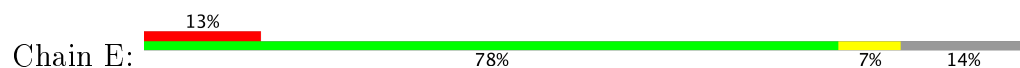


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

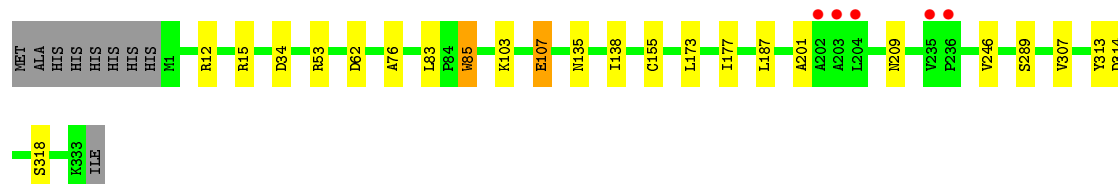
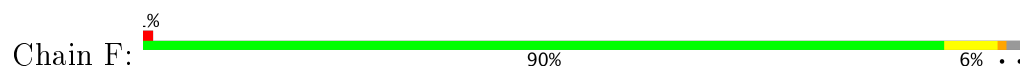




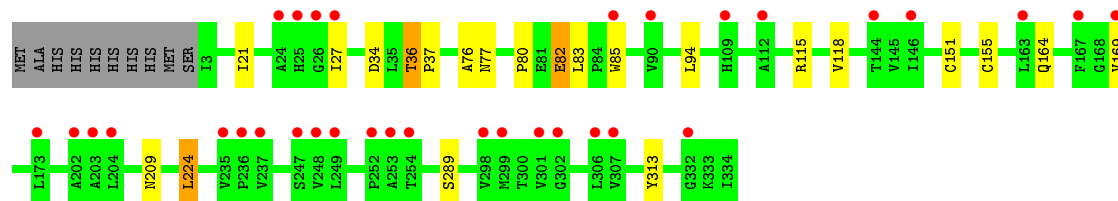
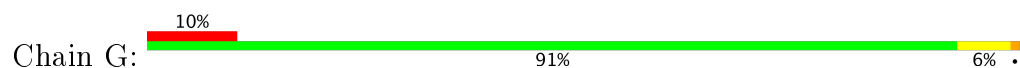
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



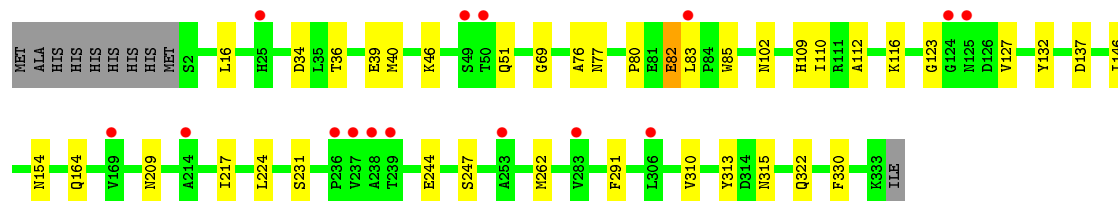
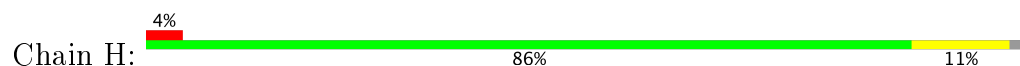
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.45Å 132.10Å 156.00Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	45.48 – 2.50 45.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.48-2.50) 99.8 (45.49-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.165 , 0.219 0.157 , 0.217	Depositor DCC
R_{free} test set	1995 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20034	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/2514	0.63	1/3415 (0.0%)
1	B	0.45	0/2517	0.62	0/3417
1	C	0.37	0/2342	0.57	0/3191
1	D	0.41	0/2513	0.61	0/3415
1	E	0.37	0/2099	0.59	0/2858
1	F	0.42	0/2527	0.60	0/3433
1	G	0.34	0/2388	0.56	0/3258
1	H	0.40	1/2418 (0.0%)	0.58	0/3301
All	All	0.40	1/19318 (0.0%)	0.60	1/26288 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	82	GLU	C-N	5.01	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	NE-CZ-NH2	-5.97	117.31	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2477	0	2465	27	0
1	B	2480	0	2472	13	0
1	C	2308	0	2174	21	0
1	D	2475	0	2458	21	0
1	E	2073	0	1919	15	0
1	F	2484	0	2471	11	0
1	G	2352	0	2188	11	0
1	H	2381	0	2265	19	0
2	A	44	0	26	2	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	0	0
2	E	44	0	26	3	0
2	F	44	0	26	0	0
2	G	44	0	26	2	0
2	H	44	0	26	1	0
3	A	2	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	111	0	0	2	0
4	B	129	0	0	0	0
4	C	60	0	0	2	0
4	D	113	0	0	2	0
4	E	52	0	0	0	0
4	F	118	0	0	0	0
4	G	21	0	0	0	0
4	H	42	0	0	1	0
All	All	20034	0	18620	131	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 3.

All (131) 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)
2:G:401:NAD:N7N	2:G:401:NAD:O2N	2.20	0.74
1:A:81:GLU:OE2	1:A:111:ARG:NH2	2.16	0.73
1:H:154:ASN:OD1	1:H:322:GLN:HG2	1.94	0.67
1:A:155:CYS:HA	1:A:289:SER:HB2	1.77	0.65
1:H:132:TYR:O	1:H:322:GLN:NE2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:O	4:A:501:HOH:O	2.16	0.61
1:C:308:LYS:HE2	3:C:402:CL:CL	2.37	0.61
1:A:61:LYS:NZ	1:A:71:GLU:OE2	2.34	0.61
1:C:155:CYS:HA	1:C:289:SER:HB2	1.83	0.60
1:H:36:THR:HG21	1:H:40:MET:HG2	1.84	0.59
1:G:34:ASP:O	1:G:76:ALA:HA	2.03	0.59
1:G:155:CYS:HA	1:G:289:SER:HB2	1.85	0.58
1:A:81:GLU:OE1	4:A:502:HOH:O	2.16	0.57
1:G:164:GLN:HB2	1:G:224:LEU:HD11	1.87	0.57
1:G:77:ASN:HD21	1:G:82:GLU:HB2	1.70	0.56
1:H:34:ASP:O	1:H:76:ALA:HA	2.07	0.55
1:A:34:ASP:O	1:A:76:ALA:HA	2.07	0.55
1:B:282:VAL:HG22	1:B:285:ILE:HD13	1.87	0.55
1:A:36:THR:HG21	1:A:40:MET:HG2	1.89	0.55
1:E:224:LEU:HA	1:E:227:LYS:HD2	1.88	0.54
1:B:115:ARG:O	1:B:116:LYS:HD3	2.07	0.54
1:A:69:GLY:HA2	1:H:69:GLY:O	2.07	0.54
1:D:215:LYS:NZ	4:D:502:HOH:O	2.33	0.54
1:E:155:CYS:HA	1:E:289:SER:HB2	1.89	0.54
1:B:34:ASP:O	1:B:76:ALA:HA	2.09	0.53
2:C:401:NAD:O2N	2:C:401:NAD:N7N	2.38	0.53
1:A:83:LEU:HD13	1:A:85:TRP:CZ2	2.44	0.53
1:C:329:TYR:CZ	1:C:333:LYS:HE3	2.44	0.52
1:A:116:LYS:NZ	1:A:143:GLU:O	2.42	0.52
1:B:155:CYS:HA	1:B:289:SER:HB2	1.92	0.52
1:D:262:MET:HG3	1:D:291:PHE:CZ	2.45	0.52
1:H:127:VAL:HG13	1:H:146:ILE:HA	1.92	0.52
1:C:95:GLU:OE1	1:C:109:HIS:NE2	2.39	0.52
1:B:36:THR:HG21	1:B:40:MET:HG2	1.93	0.51
1:F:34:ASP:O	1:F:76:ALA:HA	2.11	0.50
1:A:181:THR:OG1	1:A:183:ASP:OD1	2.27	0.50
1:C:206:ILE:HB	1:D:279:SER:HB3	1.94	0.49
1:C:329:TYR:CE2	1:C:333:LYS:HE3	2.48	0.49
1:H:164:GLN:HE21	1:H:224:LEU:HD23	1.78	0.48
1:D:83:LEU:HD13	1:D:85:TRP:CZ2	2.48	0.48
1:F:187:LEU:HA	1:F:201:ALA:HB2	1.95	0.48
1:B:80:PRO:HB3	1:B:109:HIS:CE1	2.48	0.48
1:D:3:ILE:HD13	1:D:331:ALA:HB1	1.96	0.47
1:F:103:LYS:HE2	1:F:107:GLU:OE2	2.14	0.47
1:D:34:ASP:O	1:D:76:ALA:HA	2.15	0.47
1:E:151:CYS:H	2:E:401:NAD:H5N	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLY:HA3	2:A:401:NAD:O5B	2.15	0.46
1:B:83:LEU:HD13	1:B:85:TRP:CZ2	2.50	0.46
1:H:315:ASN:O	2:H:401:NAD:H4N	2.14	0.46
1:C:181:THR:OG1	1:C:183:ASP:OD1	2.33	0.46
1:C:276:GLN:NE2	4:C:504:HOH:O	2.47	0.46
1:D:85:TRP:CE3	1:D:85:TRP:HA	2.51	0.46
1:G:94:LEU:HD23	1:G:118:VAL:HB	1.97	0.46
1:E:181:THR:OG1	1:E:183:ASP:OD1	2.34	0.46
1:H:16:LEU:HD11	1:H:51:GLN:HG3	1.98	0.46
1:C:228:LEU:C	1:D:299:MET:HE1	2.36	0.46
1:E:34:ASP:OD1	2:E:401:NAD:H1B	2.15	0.46
1:H:102:ASN:HA	1:H:123:GLY:O	2.15	0.46
1:D:174:MET:HG2	1:D:175:THR:N	2.31	0.46
1:G:164:GLN:HE22	1:G:169:VAL:H	1.63	0.45
1:F:314:ASP:O	1:F:318:SER:HB2	2.16	0.45
1:H:83:LEU:O	1:H:112:ALA:HB1	2.16	0.45
1:A:221:ILE:HG22	1:A:223:GLU:HG2	1.97	0.45
1:C:276:GLN:HG3	1:D:196:LEU:HD12	1.96	0.45
1:D:80:PRO:HB3	1:D:109:HIS:CE1	2.51	0.45
1:F:83:LEU:HD13	1:F:85:TRP:CZ2	2.51	0.45
1:A:206:ILE:HB	1:B:279:SER:HB3	1.99	0.45
1:A:110:ILE:CD1	1:A:144:THR:HB	2.47	0.45
1:A:36:THR:HG21	1:C:190:PRO:HB3	1.99	0.44
1:D:85:TRP:HA	1:D:85:TRP:HE3	1.82	0.44
1:E:12:ARG:HH21	1:E:316:GLU:CD	2.20	0.44
1:E:262:MET:HG3	1:E:291:PHE:CE1	2.52	0.44
1:B:282:VAL:HG21	1:B:312:TRP:HB3	2.00	0.44
1:F:246:VAL:HA	1:F:307:VAL:O	2.17	0.44
1:F:173:LEU:HA	1:F:173:LEU:HD23	1.79	0.44
1:H:116:LYS:HD3	1:H:330:PHE:CZ	2.52	0.44
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.82	0.44
1:C:39:GLU:HG2	4:C:548:HOH:O	2.18	0.44
1:G:151:CYS:HB3	2:G:401:NAD:H5N	2.00	0.43
1:E:262:MET:HG3	1:E:291:PHE:CZ	2.53	0.43
1:H:36:THR:CG2	1:H:40:MET:HB3	2.49	0.43
1:F:12:ARG:HH11	1:F:15:ARG:NH2	2.16	0.43
1:D:197:ARG:HB3	1:D:207:VAL:HG13	2.01	0.43
1:A:315:ASN:O	2:A:401:NAD:H4N	2.18	0.43
1:B:246:VAL:HA	1:B:307:VAL:O	2.19	0.43
1:B:255:LYS:HE3	1:B:296:THR:HB	2.00	0.43
1:D:276:GLN:NE2	4:D:505:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:CD2	1:D:78:PRO:HB3	2.49	0.43
1:G:164:GLN:NE2	1:G:169:VAL:H	2.16	0.42
1:C:239:THR:HG23	1:C:283:VAL:HG22	2.01	0.42
1:E:233:GLN:HG3	1:F:177:ILE:CD1	2.48	0.42
1:H:262:MET:HG3	1:H:291:PHE:CE1	2.54	0.42
1:A:91:ASP:OD1	1:A:115:ARG:NH1	2.52	0.42
1:C:34:ASP:O	1:C:76:ALA:HA	2.19	0.42
1:E:314:ASP:O	1:E:318:SER:HB2	2.19	0.42
1:C:164:GLN:HB2	1:C:224:LEU:HD21	2.01	0.42
1:D:204:LEU:HA	1:D:204:LEU:HD23	1.89	0.42
1:G:21:ILE:HG23	1:G:27:ILE:HG23	2.01	0.42
1:A:314:ASP:O	1:A:318:SER:HB2	2.19	0.42
1:E:135:ASN:O	1:E:138:ILE:HG12	2.20	0.42
1:A:110:ILE:HD13	1:A:144:THR:HB	2.02	0.42
1:C:94:LEU:HD23	1:C:94:LEU:HA	1.89	0.42
1:H:36:THR:HG21	1:H:40:MET:CG	2.48	0.41
1:A:103:LYS:HE2	1:A:107:GLU:OE2	2.19	0.41
1:A:224:LEU:HA	1:A:227:LYS:HD2	2.02	0.41
1:C:83:LEU:HA	1:C:84:PRO:HD3	1.85	0.41
1:A:272:TYR:CE2	1:A:274:GLU:HG3	2.56	0.41
1:D:81:GLU:OE2	1:D:111:ARG:NH2	2.45	0.41
1:E:246:VAL:HA	1:E:307:VAL:O	2.21	0.41
1:F:135:ASN:O	1:F:138:ILE:HG12	2.21	0.41
1:G:80:PRO:HA	1:G:83:LEU:HD12	2.01	0.41
1:H:80:PRO:HB3	1:H:109:HIS:CE1	2.55	0.41
1:E:151:CYS:SG	2:E:401:NAD:H4N	2.61	0.41
1:A:116:LYS:HD3	1:A:330:PHE:CZ	2.56	0.41
1:H:46:LYS:HE3	4:H:539:HOH:O	2.20	0.41
1:D:181:THR:OG1	1:D:183:ASP:OD1	2.37	0.41
1:D:223:GLU:H	1:D:223:GLU:CD	2.24	0.41
1:C:299:MET:HE1	1:D:228:LEU:C	2.41	0.41
1:H:77:ASN:HD21	1:H:82:GLU:CD	2.24	0.41
1:E:178:HIS:O	1:E:234:ARG:HA	2.21	0.41
1:F:155:CYS:HA	1:F:289:SER:HB2	2.03	0.41
1:H:244:GLU:HG2	1:H:310:VAL:HG22	2.03	0.41
1:D:217:ILE:HG23	1:D:221:ILE:HD12	2.03	0.40
1:B:207:VAL:HB	1:B:234:ARG:HB2	2.02	0.40
1:C:10:PHE:CE1	1:C:32:VAL:HG11	2.56	0.40
1:E:173:LEU:HA	1:E:173:LEU:HD23	1.93	0.40
1:A:262:MET:HG3	1:A:291:PHE:CZ	2.57	0.40
1:G:36:THR:HG23	1:G:37:PRO:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ILE:O	1:C:262:MET:HG2	2.20	0.40
1:A:233:GLN:HG3	1:B:177:ILE:CD1	2.51	0.40
1:C:151:CYS:HB3	2:C:401:NAD:H5N	2.03	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	331/342 (97%)	321 (97%)	10 (3%)	0	100	100
1	B	332/342 (97%)	324 (98%)	8 (2%)	0	100	100
1	C	321/342 (94%)	312 (97%)	9 (3%)	0	100	100
1	D	332/342 (97%)	320 (96%)	12 (4%)	0	100	100
1	E	285/342 (83%)	277 (97%)	8 (3%)	0	100	100
1	F	333/342 (97%)	322 (97%)	10 (3%)	1 (0%)	44	66
1	G	330/342 (96%)	318 (96%)	12 (4%)	0	100	100
1	H	330/342 (96%)	321 (97%)	9 (3%)	0	100	100
All	All	2594/2736 (95%)	2515 (97%)	78 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	62	ASP

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	259/273 (95%)	253 (98%)	6 (2%)	56	81
1	B	258/273 (94%)	250 (97%)	8 (3%)	45	73
1	C	220/273 (81%)	214 (97%)	6 (3%)	50	77
1	D	257/273 (94%)	252 (98%)	5 (2%)	62	85
1	E	198/273 (72%)	195 (98%)	3 (2%)	70	89
1	F	259/273 (95%)	253 (98%)	6 (2%)	56	81
1	G	223/273 (82%)	216 (97%)	7 (3%)	45	73
1	H	234/273 (86%)	225 (96%)	9 (4%)	38	64
All	All	1908/2184 (87%)	1858 (97%)	50 (3%)	51	78

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	61	LYS
1	A	62	ASP
1	A	85	TRP
1	A	209	ASN
1	A	313	TYR
1	B	2	SER
1	B	36	THR
1	B	85	TRP
1	B	165	LYS
1	B	209	ASN
1	B	211	THR
1	B	282	VAL
1	B	313	TYR
1	C	70	ARG
1	C	91	ASP
1	C	101	THR
1	C	209	ASN
1	C	308	LYS
1	C	313	TYR
1	D	2	SER
1	D	36	THR
1	D	85	TRP
1	D	211	THR

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Mol	Chain	Res	Type
1	D	313	TYR
1	E	209	ASN
1	E	313	TYR
1	E	326	THR
1	F	53[A]	ARG
1	F	53[B]	ARG
1	F	85	TRP
1	F	107	GLU
1	F	209	ASN
1	F	313	TYR
1	G	36	THR
1	G	82	GLU
1	G	85	TRP
1	G	115	ARG
1	G	209	ASN
1	G	224	LEU
1	G	313	TYR
1	H	39	GLU
1	H	85	TRP
1	H	110	ILE
1	H	137	ASP
1	H	209	ASN
1	H	217	ILE
1	H	231	SER
1	H	247	SER
1	H	313	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	GLN
1	G	164	GLN
1	H	164	GLN

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 14 ligands modelled in this entry, 6 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	$\# Z > 2$
2	NAD	A	401	-	41,48,48	0.50	0	43,73,73	0.63	0
2	NAD	B	401	-	41,48,48	0.58	0	43,73,73	0.66	0
2	NAD	C	401	-	41,48,48	0.54	0	43,73,73	0.63	1 (2%)
2	NAD	D	401	-	41,48,48	0.53	0	43,73,73	0.70	0
2	NAD	E	401	-	41,48,48	0.55	0	43,73,73	0.63	0
2	NAD	F	401	-	41,48,48	0.49	0	43,73,73	0.77	0
2	NAD	G	401	-	41,48,48	0.54	0	43,73,73	0.57	0
2	NAD	H	401	-	41,48,48	0.48	0	43,73,73	0.65	0

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	401	-	-	0/22/62/62	0/5/5/5
2	NAD	B	401	-	-	0/22/62/62	0/5/5/5
2	NAD	C	401	-	-	0/22/62/62	0/5/5/5
2	NAD	D	401	-	-	0/22/62/62	0/5/5/5
2	NAD	E	401	-	-	0/22/62/62	0/5/5/5
2	NAD	F	401	-	-	0/22/62/62	0/5/5/5
2	NAD	G	401	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	H	401	-	-	0/22/62/62	0/5/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	401	NAD	O5B-PA-O1A	2.15	117.91	109.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	2	0
2	C	401	NAD	2	0
2	E	401	NAD	3	0
2	G	401	NAD	2	0
2	H	401	NAD	1	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, 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	333/342 (97%)	-0.27	3 (0%) 84 85	24, 38, 62, 85	0
1	B	334/342 (97%)	-0.46	1 (0%) 93 94	26, 37, 58, 90	0
1	C	325/342 (95%)	0.48	41 (12%) 4 3	27, 58, 112, 140	0
1	D	334/342 (97%)	-0.18	1 (0%) 93 94	25, 43, 68, 108	0
1	E	293/342 (85%)	0.52	44 (15%) 3 2	31, 56, 113, 145	0
1	F	333/342 (97%)	-0.39	5 (1%) 74 75	27, 38, 60, 101	0
1	G	332/342 (97%)	0.46	33 (9%) 8 7	47, 76, 103, 123	0
1	H	332/342 (97%)	0.11	15 (4%) 34 36	37, 67, 100, 115	0
All	All	2616/2736 (95%)	0.02	143 (5%) 26 27	24, 49, 100, 145	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	145	VAL	7.8
1	E	29	VAL	7.5
1	E	30	ALA	7.1
1	C	32	VAL	6.6
1	C	24	ALA	5.9
1	G	249	LEU	5.7
1	G	26	GLY	5.6
1	E	67	VAL	5.3
1	E	99	PHE	5.2
1	G	27	ILE	5.2
1	E	32	VAL	5.1
1	E	21	ILE	5.0
1	E	71	GLU	5.0
1	E	58	ALA	5.0
1	C	104	THR	4.9
1	C	144	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	85	TRP	4.8
1	G	163	LEU	4.7
1	C	145	VAL	4.6
1	E	125	ASN	4.5
1	E	31	ALA	4.5
1	E	104	THR	4.4
1	H	306	LEU	4.4
1	E	7	ILE	4.2
1	E	66	VAL	4.2
1	E	100	PHE	4.2
1	E	144	THR	4.1
1	C	109	HIS	4.1
1	E	98	GLY	4.0
1	E	57	THR	4.0
1	G	253	ALA	3.9
1	C	106	ALA	3.8
1	E	330	PHE	3.7
1	C	29	VAL	3.7
1	E	38	ALA	3.7
1	C	64	ALA	3.7
1	C	75	PHE	3.7
1	C	116	LYS	3.6
1	G	236	PRO	3.6
1	C	30	ALA	3.6
1	C	92	VAL	3.6
1	C	65	ILE	3.6
1	E	24	ALA	3.6
1	G	247	SER	3.5
1	G	25	HIS	3.5
1	E	74	VAL	3.5
1	G	144	THR	3.4
1	E	72	ILE	3.3
1	G	167	PHE	3.3
1	C	72	ILE	3.3
1	C	6	ALA	3.2
1	H	237	VAL	3.2
1	G	169	VAL	3.2
1	C	117	VAL	3.2
1	C	146	ILE	3.2
1	E	56	GLY	3.1
1	E	27	ILE	3.1
1	C	83	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	254	THR	3.0
1	G	204	LEU	3.0
1	G	252	PRO	3.0
1	C	93	VAL	3.0
1	G	298	VAL	3.0
1	C	31	ALA	3.0
1	G	203	ALA	2.9
1	G	235	VAL	2.9
1	G	202	ALA	2.8
1	F	203	ALA	2.8
1	E	8	ASN	2.8
1	C	74	VAL	2.8
1	G	307	VAL	2.8
1	H	236	PRO	2.8
1	E	73	LYS	2.8
1	C	125	ASN	2.8
1	E	60	LEU	2.7
1	E	28	GLU	2.7
1	E	33	ASN	2.6
1	C	330	PHE	2.6
1	E	68	ASN	2.6
1	E	42	LEU	2.5
1	C	62	ASP	2.5
1	G	332	GLY	2.5
1	E	331	ALA	2.5
1	A	237	VAL	2.5
1	G	248	VAL	2.5
1	G	109	HIS	2.5
1	C	130	VAL	2.4
1	G	146	ILE	2.4
1	G	173	LEU	2.4
1	E	146	ILE	2.4
1	D	237	VAL	2.4
1	F	236	PRO	2.4
1	F	204	LEU	2.4
1	E	124	GLY	2.4
1	H	125	ASN	2.4
1	C	264	ALA	2.4
1	H	239	THR	2.4
1	G	237	VAL	2.3
1	G	24	ALA	2.3
1	E	97	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	106	ALA	2.3
1	B	25	HIS	2.3
1	C	108	ALA	2.3
1	C	60	LEU	2.3
1	H	49	SER	2.3
1	C	326	THR	2.3
1	C	91	ASP	2.2
1	C	25	HIS	2.2
1	G	302	GLY	2.2
1	E	127	VAL	2.2
1	F	202	ALA	2.2
1	H	50	THR	2.2
1	C	205	ASN	2.2
1	C	114	ALA	2.2
1	E	237	VAL	2.2
1	A	238	ALA	2.2
1	G	306	LEU	2.2
1	G	301	VAL	2.2
1	E	202	ALA	2.2
1	H	124	GLY	2.2
1	C	4	LYS	2.2
1	G	112	ALA	2.2
1	H	214	ALA	2.2
1	H	238	ALA	2.2
1	H	25	HIS	2.1
1	C	63	ASP	2.1
1	H	83	LEU	2.1
1	C	139	LEU	2.1
1	E	35	LEU	2.1
1	C	236	PRO	2.1
1	G	299	MET	2.1
1	C	203	ALA	2.1
1	F	235	VAL	2.1
1	H	169	VAL	2.1
1	H	283	VAL	2.1
1	E	139	LEU	2.1
1	A	1	MET	2.1
1	H	253	ALA	2.1
1	G	90	VAL	2.1
1	E	59	GLU	2.0
1	C	70	ARG	2.0
1	E	238	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	333	LYS	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CL	A	402	1/1	0.99	0.15	0.81	39,39,39,39	0
2	NAD	C	401	44/44	0.91	0.17	0.04	60,72,83,85	0
2	NAD	G	401	44/44	0.93	0.15	0.03	32,63,97,99	0
2	NAD	E	401	44/44	0.88	0.19	-0.14	47,79,85,88	44
2	NAD	B	401	44/44	0.98	0.12	-0.17	20,30,35,39	0
3	CL	C	402	1/1	0.98	0.14	-0.20	56,56,56,56	0
2	NAD	D	401	44/44	0.97	0.12	-0.52	31,37,42,45	0
2	NAD	F	401	44/44	0.98	0.11	-0.67	25,36,45,49	0
2	NAD	H	401	44/44	0.96	0.12	-0.80	35,52,61,67	0
2	NAD	A	401	44/44	0.97	0.13	-0.86	33,44,54,56	0
3	CL	E	402	1/1	0.99	0.10	-1.48	40,40,40,40	0
3	CL	A	403	1/1	0.97	0.09	-1.93	59,59,59,59	0
3	CL	D	402	1/1	0.98	0.08	-2.06	47,47,47,47	0
3	CL	F	402	1/1	0.98	0.09	-2.94	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.