



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:56 PM GMT

PDB ID : 1VSV
Title : Crystal Structure of holo-glyceraldehyde 3-phosphate dehydrogenase from *Cryptosporidium parvum*
Authors : Cook, W.J.; Senkovich, O.; Chattopadhyay, D.
Deposited on : 2008-03-11
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

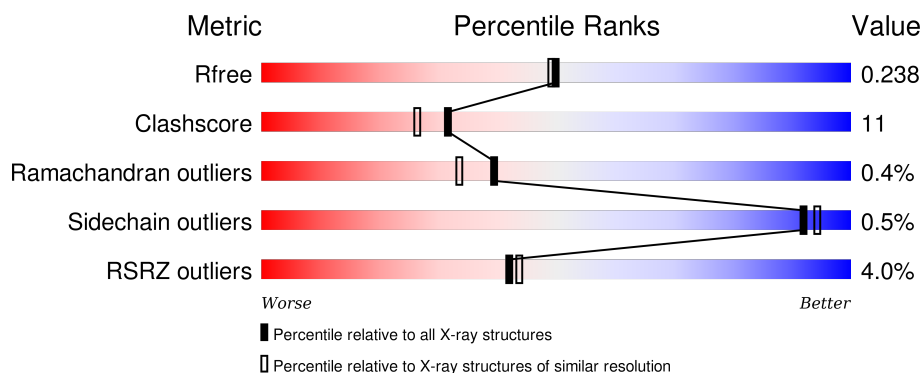
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	359	<div> <div>0%</div> <div>76% 18% • 6%</div> </div>
1	B	359	<div> <div>4%</div> <div>74% 19% • 6%</div> </div>
1	C	359	<div> <div>8%</div> <div>74% 20% 6%</div> </div>
1	D	359	<div> <div>2%</div> <div>76% 18% • 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10679 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	338	Total	C	N	O	S	0	0	0
			2521	1592	425	486	18			
1	B	338	Total	C	N	O	S	0	0	0
			2521	1592	425	486	18			
1	C	338	Total	C	N	O	S	0	0	0
			2521	1592	425	486	18			
1	D	338	Total	C	N	O	S	0	0	0
			2521	1592	425	486	18			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q7YYQ9
A	-18	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
A	-17	SER	-	EXPRESSION TAG	UNP Q7YYQ9
A	-16	SER	-	EXPRESSION TAG	UNP Q7YYQ9
A	-15	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
A	-14	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
A	-13	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
A	-12	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
A	-11	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
A	-10	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
A	-9	SER	-	EXPRESSION TAG	UNP Q7YYQ9
A	-8	SER	-	EXPRESSION TAG	UNP Q7YYQ9
A	-7	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
A	-6	LEU	-	EXPRESSION TAG	UNP Q7YYQ9
A	-5	VAL	-	EXPRESSION TAG	UNP Q7YYQ9
A	-4	PRO	-	EXPRESSION TAG	UNP Q7YYQ9
A	-3	ARG	-	EXPRESSION TAG	UNP Q7YYQ9
A	-2	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
A	-1	SER	-	EXPRESSION TAG	UNP Q7YYQ9
A	0	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
B	-19	MET	-	EXPRESSION TAG	UNP Q7YYQ9

Continued on next page...

Continued from previous page...

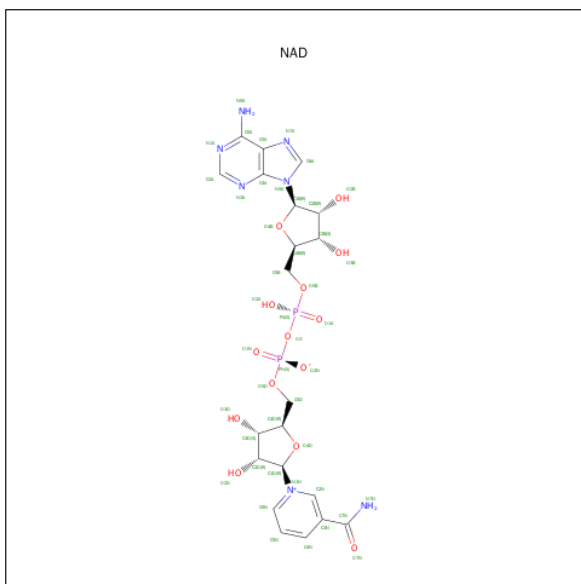
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
B	-17	SER	-	EXPRESSION TAG	UNP Q7YYQ9
B	-16	SER	-	EXPRESSION TAG	UNP Q7YYQ9
B	-15	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
B	-14	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
B	-13	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
B	-12	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
B	-11	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
B	-10	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
B	-9	SER	-	EXPRESSION TAG	UNP Q7YYQ9
B	-8	SER	-	EXPRESSION TAG	UNP Q7YYQ9
B	-7	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
B	-6	LEU	-	EXPRESSION TAG	UNP Q7YYQ9
B	-5	VAL	-	EXPRESSION TAG	UNP Q7YYQ9
B	-4	PRO	-	EXPRESSION TAG	UNP Q7YYQ9
B	-3	ARG	-	EXPRESSION TAG	UNP Q7YYQ9
B	-2	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
B	-1	SER	-	EXPRESSION TAG	UNP Q7YYQ9
B	0	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
C	-19	MET	-	EXPRESSION TAG	UNP Q7YYQ9
C	-18	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
C	-17	SER	-	EXPRESSION TAG	UNP Q7YYQ9
C	-16	SER	-	EXPRESSION TAG	UNP Q7YYQ9
C	-15	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
C	-14	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
C	-13	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
C	-12	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
C	-11	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
C	-10	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
C	-9	SER	-	EXPRESSION TAG	UNP Q7YYQ9
C	-8	SER	-	EXPRESSION TAG	UNP Q7YYQ9
C	-7	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
C	-6	LEU	-	EXPRESSION TAG	UNP Q7YYQ9
C	-5	VAL	-	EXPRESSION TAG	UNP Q7YYQ9
C	-4	PRO	-	EXPRESSION TAG	UNP Q7YYQ9
C	-3	ARG	-	EXPRESSION TAG	UNP Q7YYQ9
C	-2	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
C	-1	SER	-	EXPRESSION TAG	UNP Q7YYQ9
C	0	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
D	-19	MET	-	EXPRESSION TAG	UNP Q7YYQ9
D	-18	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
D	-17	SER	-	EXPRESSION TAG	UNP Q7YYQ9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP Q7YYQ9
D	-15	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
D	-14	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
D	-13	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
D	-12	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
D	-11	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
D	-10	HIS	-	EXPRESSION TAG	UNP Q7YYQ9
D	-9	SER	-	EXPRESSION TAG	UNP Q7YYQ9
D	-8	SER	-	EXPRESSION TAG	UNP Q7YYQ9
D	-7	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
D	-6	LEU	-	EXPRESSION TAG	UNP Q7YYQ9
D	-5	VAL	-	EXPRESSION TAG	UNP Q7YYQ9
D	-4	PRO	-	EXPRESSION TAG	UNP Q7YYQ9
D	-3	ARG	-	EXPRESSION TAG	UNP Q7YYQ9
D	-2	GLY	-	EXPRESSION TAG	UNP Q7YYQ9
D	-1	SER	-	EXPRESSION TAG	UNP Q7YYQ9
D	0	HIS	-	EXPRESSION TAG	UNP Q7YYQ9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

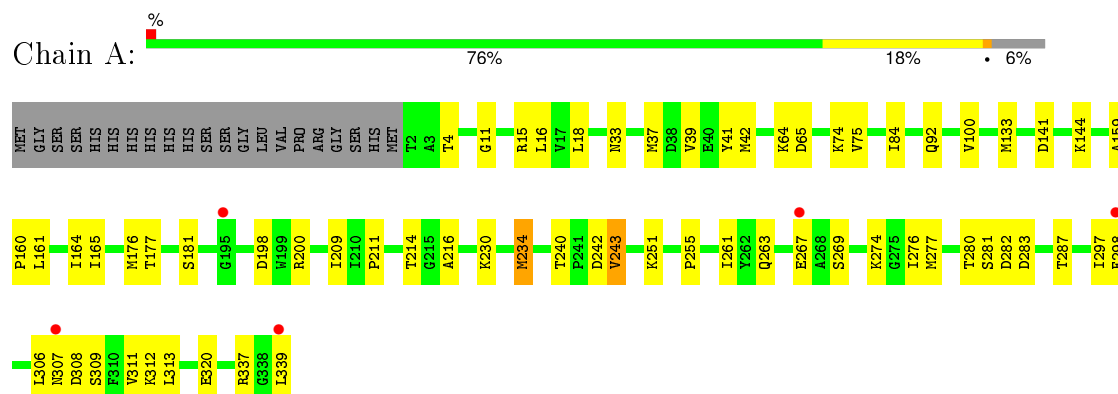
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	104	Total	O	0	0
			104	104		
3	C	78	Total	O	0	0
			78	78		
3	D	137	Total	O	0	0
			137	137		

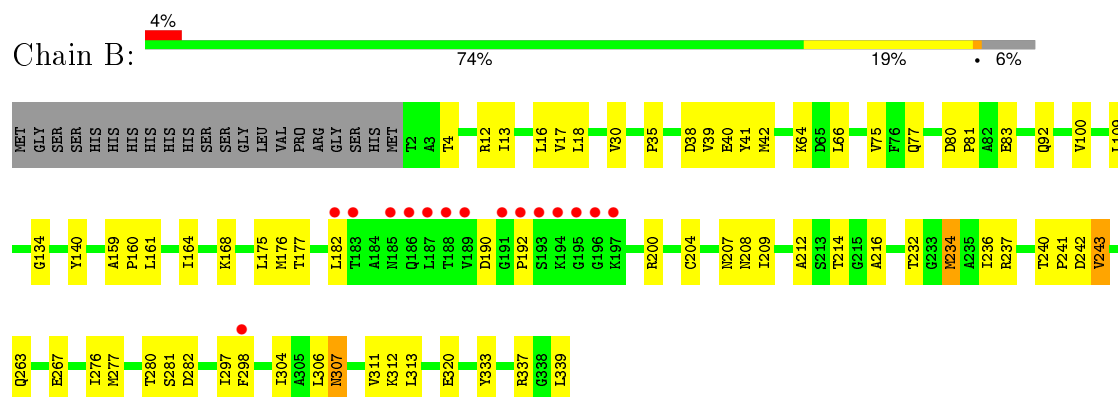
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

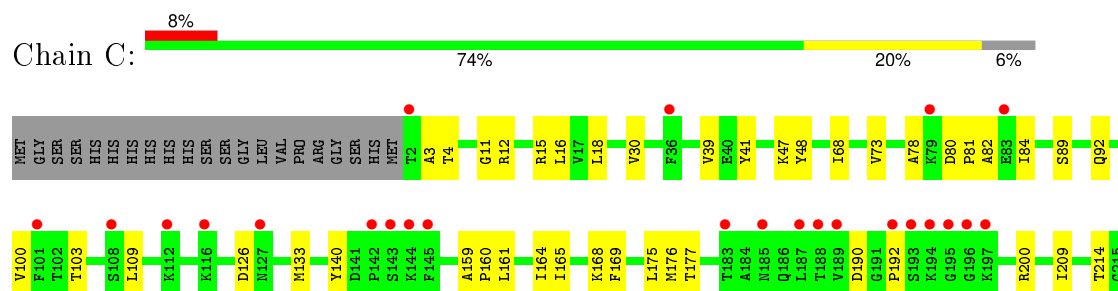
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

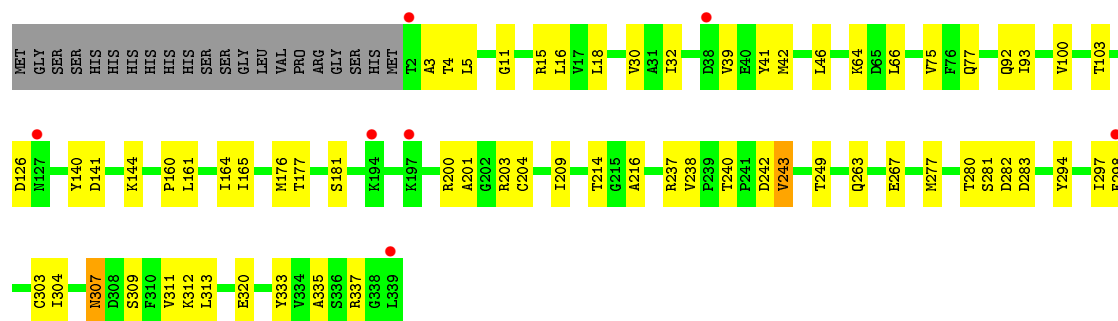
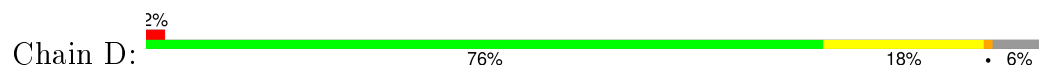


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





● Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.12Å 121.19Å 80.33Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	48.85 – 2.00 48.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.85-2.00) 98.2 (48.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.205 , 0.238 0.205 , 0.238	Depositor DCC
R_{free} test set	4419 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.0	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 87579 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10679	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.31	0/2565	0.59	1/3478 (0.0%)
1	B	0.31	0/2565	0.60	1/3478 (0.0%)
1	C	0.30	0/2565	0.58	1/3478 (0.0%)
1	D	0.32	0/2565	0.62	1/3478 (0.0%)
All	All	0.31	0/10260	0.60	4/13912 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	209	ILE	N-CA-C	-6.18	94.31	111.00
1	A	209	ILE	N-CA-C	-5.92	95.01	111.00
1	B	209	ILE	N-CA-C	-5.70	95.62	111.00
1	C	209	ILE	N-CA-C	-5.61	95.84	111.00

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	2521	0	2545	52	0
1	B	2521	0	2545	71	0
1	C	2521	0	2545	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2521	0	2545	51	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	100	0	0	4	0
3	B	104	0	0	1	0
3	C	78	0	0	2	0
3	D	137	0	0	3	0
All	All	10679	0	10284	220	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 11.

All (220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:THR:HG22	1:D:282:ASP:H	1.28	0.98
1:A:280:THR:HG22	1:A:282:ASP:H	1.30	0.96
1:B:280:THR:HG22	1:B:282:ASP:H	1.31	0.94
1:D:307:ASN:HD22	1:D:309:SER:H	1.20	0.86
1:C:280:THR:HG22	1:C:282:ASP:H	1.40	0.85
1:B:337:ARG:HH11	1:B:337:ARG:HG2	1.43	0.84
1:D:214:THR:HG22	1:D:216:ALA:H	1.40	0.84
1:B:214:THR:HG22	1:B:216:ALA:H	1.44	0.82
1:A:161:LEU:N	1:A:277:MET:HE1	1.98	0.77
1:B:12:ARG:NH1	1:C:190:ASP:HB2	2.01	0.75
1:A:200:ARG:NH1	1:A:211:PRO:HB2	2.02	0.74
1:D:164:ILE:HD12	1:D:277:MET:HE3	1.69	0.74
1:C:161:LEU:N	1:C:277:MET:HE1	2.04	0.72
1:A:200:ARG:HH11	1:A:211:PRO:HB2	1.52	0.72
1:A:164:ILE:HD12	1:A:277:MET:HE3	1.71	0.72
1:D:39:VAL:HG23	3:D:469:HOH:O	1.90	0.71
1:B:39:VAL:HG21	1:B:64:LYS:O	1.90	0.70
1:A:214:THR:HG22	1:A:216:ALA:H	1.56	0.70
1:A:337:ARG:NH2	1:A:337:ARG:HB3	2.07	0.69
1:A:234:MET:HG2	1:B:304:ILE:HD13	1.73	0.69
1:D:307:ASN:ND2	1:D:309:SER:H	1.89	0.69
1:C:263:GLN:O	1:C:267:GLU:HG2	1.93	0.69
1:B:160:PRO:HB2	1:B:277:MET:HE1	1.74	0.69
1:B:190:ASP:HB2	1:C:12:ARG:NH1	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLN:O	1:D:267:GLU:HG2	1.93	0.68
1:A:200:ARG:CZ	3:A:454:HOH:O	2.40	0.68
1:D:201:ALA:HB2	1:D:237:ARG:HH12	1.57	0.68
1:C:160:PRO:HB3	1:C:273:MET:HE1	1.75	0.68
1:D:161:LEU:N	1:D:277:MET:HE1	2.08	0.68
1:B:164:ILE:HD12	1:B:277:MET:HE3	1.76	0.67
1:C:214:THR:HG22	1:C:216:ALA:H	1.58	0.67
1:B:41:TYR:CE2	1:C:192:PRO:HA	2.30	0.66
1:B:263:GLN:O	1:B:267:GLU:HG2	1.95	0.66
1:C:176:MET:HG2	1:C:177:THR:N	2.11	0.65
1:A:176:MET:HG2	1:A:177:THR:N	2.11	0.65
1:D:4:THR:OG1	1:D:92:GLN:HG3	1.97	0.64
1:B:333:TYR:CZ	1:B:337:ARG:HD2	2.33	0.64
1:D:176:MET:HG2	1:D:177:THR:N	2.12	0.64
1:B:192:PRO:HA	1:C:41:TYR:OH	1.97	0.63
1:B:306:LEU:HG	1:B:307:ASN:OD1	1.99	0.63
1:B:176:MET:HG2	1:B:177:THR:N	2.14	0.63
1:C:175:LEU:HD12	1:D:249:THR:HG23	1.81	0.63
1:B:12:ARG:HH11	1:C:190:ASP:HB2	1.62	0.62
1:D:311:VAL:HG12	1:D:312:LYS:N	2.13	0.62
1:D:39:VAL:HG22	1:D:75:VAL:HG11	1.82	0.61
1:B:39:VAL:HG22	1:B:75:VAL:HG11	1.82	0.61
1:C:47:LYS:HG3	1:C:48:TYR:CD2	2.36	0.61
1:C:4:THR:OG1	1:C:92:GLN:HG3	2.01	0.61
1:B:40:GLU:H	1:B:40:GLU:CD	2.04	0.61
1:A:337:ARG:HH21	1:A:337:ARG:HB3	1.66	0.61
1:A:16:LEU:HD12	1:A:320:GLU:HB3	1.82	0.61
1:A:181:SER:HB2	1:A:240:THR:O	2.01	0.61
1:B:41:TYR:HE2	1:C:192:PRO:HA	1.65	0.60
1:D:16:LEU:HD12	1:D:320:GLU:HB3	1.84	0.60
1:B:337:ARG:NH1	1:B:337:ARG:HG2	2.14	0.59
1:D:164:ILE:HD12	1:D:277:MET:CE	2.32	0.59
1:B:4:THR:OG1	1:B:92:GLN:HG3	2.02	0.59
1:C:39:VAL:HG23	3:C:571:HOH:O	2.01	0.59
1:D:181:SER:HB2	1:D:240:THR:O	2.01	0.59
1:C:30:VAL:HG11	1:C:89:SER:O	2.02	0.59
1:C:283:ASP:HB3	1:D:200:ARG:HG2	1.85	0.59
1:A:16:LEU:CD1	1:A:320:GLU:HB3	2.33	0.59
1:B:192:PRO:HA	1:C:41:TYR:CE2	2.38	0.58
1:D:39:VAL:HG21	1:D:64:LYS:O	2.03	0.58
1:B:175:LEU:HD23	1:B:232:THR:HG23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LEU:CA	1:C:277:MET:HE1	2.34	0.58
1:C:16:LEU:CD1	1:C:320:GLU:HB3	2.35	0.57
1:B:64:LYS:HG2	1:B:64:LYS:O	2.04	0.56
1:D:201:ALA:HB2	1:D:237:ARG:NH1	2.19	0.56
1:A:159:ALA:HB3	1:A:160:PRO:HD3	1.86	0.56
1:C:68:ILE:HD12	1:C:73:VAL:HG21	1.87	0.56
1:B:311:VAL:HG12	1:B:312:LYS:N	2.20	0.56
1:B:161:LEU:N	1:B:277:MET:HE1	2.19	0.56
1:C:175:LEU:HD23	1:C:232:THR:HG22	1.88	0.56
1:B:13:ILE:O	1:B:17:VAL:HG23	2.06	0.56
1:B:38:ASP:HB3	1:B:40:GLU:OE1	2.06	0.56
1:A:311:VAL:HG12	1:A:312:LYS:N	2.21	0.56
1:B:140:TYR:HD2	1:B:337:ARG:HD3	1.71	0.55
1:B:333:TYR:CE2	1:B:337:ARG:HD2	2.41	0.55
1:D:280:THR:HG22	1:D:281:SER:N	2.22	0.55
1:A:39:VAL:HG22	1:A:75:VAL:HG11	1.89	0.55
1:A:263:GLN:O	1:A:267:GLU:HG2	2.07	0.55
1:C:164:ILE:HD12	1:C:277:MET:HE3	1.89	0.54
1:B:16:LEU:CD1	1:B:320:GLU:HB3	2.37	0.54
1:B:182:LEU:HG	1:B:240:THR:O	2.07	0.54
1:D:75:VAL:CG1	1:D:77:GLN:HE22	2.21	0.54
1:A:234:MET:HG2	1:B:304:ILE:CD1	2.36	0.54
1:D:103:THR:HA	1:D:126:ASP:OD1	2.08	0.54
1:C:140:TYR:HD2	1:C:337:ARG:HD3	1.72	0.53
1:B:42:MET:HE2	1:B:66:LEU:HD11	1.90	0.53
1:A:164:ILE:HD12	1:A:277:MET:CE	2.37	0.53
1:B:177:THR:HG23	1:B:234:MET:CE	2.39	0.53
1:C:311:VAL:HG12	1:C:312:LYS:N	2.24	0.53
1:B:168:LYS:HG2	3:B:530:HOH:O	2.09	0.53
1:B:160:PRO:C	1:B:277:MET:HE1	2.30	0.52
1:C:140:TYR:CD2	1:C:337:ARG:HD3	2.44	0.52
1:B:100:VAL:O	1:B:100:VAL:HG12	2.10	0.52
1:C:161:LEU:HA	1:C:277:MET:CE	2.40	0.52
1:C:238:VAL:HG11	1:D:238:VAL:HG11	1.91	0.52
1:D:304:ILE:O	1:D:311:VAL:HG13	2.10	0.51
1:D:100:VAL:HG12	1:D:100:VAL:O	2.09	0.51
1:C:169:PHE:O	1:C:253:ALA:HB3	2.10	0.51
1:C:133:MET:O	1:C:276:ILE:HD13	2.10	0.51
1:D:160:PRO:C	1:D:277:MET:HE1	2.31	0.51
1:C:333:TYR:CZ	1:C:337:ARG:HD2	2.46	0.51
1:A:100:VAL:HG12	1:A:100:VAL:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLY:O	1:C:15:ARG:HG3	2.11	0.51
1:C:333:TYR:CE2	1:C:337:ARG:HD2	2.46	0.51
1:C:297:ILE:HD12	1:C:297:ILE:N	2.25	0.50
1:C:103:THR:HA	1:C:126:ASP:OD1	2.11	0.50
1:A:39:VAL:HG21	1:A:64:LYS:O	2.11	0.50
1:B:177:THR:HG23	1:B:234:MET:HE1	1.94	0.50
1:C:159:ALA:HB3	1:C:160:PRO:HD3	1.93	0.50
1:A:160:PRO:C	1:A:277:MET:HE1	2.31	0.50
1:C:92:GLN:HB3	1:C:339:LEU:HD13	1.93	0.50
1:C:294:TYR:HB2	1:C:297:ILE:HD11	1.94	0.50
1:B:190:ASP:HB2	1:C:12:ARG:HH11	1.74	0.49
1:D:11:GLY:O	1:D:15:ARG:HG3	2.12	0.49
1:B:35:PRO:HB3	1:B:77:GLN:O	2.12	0.49
1:B:234:MET:CE	1:B:236:ILE:HG13	2.42	0.49
1:A:161:LEU:HA	1:A:277:MET:HE3	1.94	0.49
1:D:311:VAL:CG1	1:D:312:LYS:N	2.76	0.49
1:D:144:LYS:NZ	3:D:465:HOH:O	2.45	0.49
1:A:4:THR:OG1	1:A:92:GLN:HG3	2.13	0.48
1:B:159:ALA:HB3	1:B:160:PRO:HD3	1.94	0.48
1:A:141:ASP:OD1	1:A:144:LYS:HG3	2.12	0.48
1:D:18:LEU:CD1	1:D:32:ILE:HD11	2.43	0.48
1:A:280:THR:HG22	1:A:281:SER:N	2.29	0.48
1:A:11:GLY:HA3	2:A:340:NAD:O5B	2.13	0.48
1:B:234:MET:HE1	1:B:236:ILE:HG13	1.95	0.48
1:B:204:CYS:SG	1:B:207:ASN:OD1	2.72	0.48
1:D:3:ALA:HB2	1:D:335:ALA:CB	2.43	0.48
1:D:18:LEU:HD12	1:D:32:ILE:HD11	1.96	0.47
1:A:37:MET:HB3	1:A:42:MET:HG3	1.96	0.47
1:C:161:LEU:HA	1:C:277:MET:HE1	1.96	0.47
1:D:161:LEU:HA	1:D:277:MET:HE3	1.96	0.47
1:B:41:TYR:OH	1:C:192:PRO:HA	2.14	0.47
1:B:298:PHE:HE1	1:B:313:LEU:HB3	1.79	0.47
1:C:242:ASP:O	1:C:243:VAL:HB	2.15	0.47
1:D:161:LEU:O	1:D:165:ILE:HG12	2.15	0.47
1:B:192:PRO:HA	1:C:41:TYR:HE2	1.79	0.47
1:D:16:LEU:CD1	1:D:320:GLU:HB3	2.44	0.47
1:A:242:ASP:O	1:A:243:VAL:HB	2.15	0.47
1:A:11:GLY:O	1:A:15:ARG:HG3	2.15	0.47
1:D:5:LEU:HD12	1:D:93:ILE:O	2.15	0.46
1:C:3:ALA:HA	1:C:92:GLN:OE1	2.15	0.46
1:C:337:ARG:HH11	1:C:337:ARG:HG2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ASP:O	1:D:243:VAL:HB	2.15	0.46
1:C:164:ILE:HD12	1:C:277:MET:CE	2.45	0.46
1:B:16:LEU:HD12	1:B:320:GLU:HB3	1.98	0.46
1:B:134:GLY:HA3	1:B:276:ILE:HD13	1.97	0.46
1:C:175:LEU:CD2	1:C:232:THR:HG22	2.46	0.46
1:A:18:LEU:HD23	1:A:18:LEU:C	2.35	0.45
1:C:18:LEU:C	1:C:18:LEU:HD23	2.36	0.45
1:B:92:GLN:HB3	1:B:339:LEU:HD13	1.99	0.45
1:C:161:LEU:O	1:C:165:ILE:HG12	2.17	0.45
1:A:337:ARG:HH21	1:A:337:ARG:CB	2.28	0.45
1:C:330:LEU:O	1:C:334:VAL:HG23	2.17	0.45
1:B:192:PRO:HA	1:C:41:TYR:CZ	2.52	0.45
1:A:165:ILE:HD11	1:A:261:ILE:HG23	1.98	0.45
1:B:81:PRO:HB2	1:B:109:LEU:HB2	1.99	0.45
1:C:280:THR:HG22	1:C:281:SER:N	2.31	0.45
1:C:11:GLY:HA3	2:C:340:NAD:O5B	2.17	0.45
1:C:168:LYS:HG3	1:C:264:ALA:HB1	1.98	0.45
1:B:280:THR:HG22	1:B:281:SER:N	2.31	0.45
1:C:81:PRO:HB2	1:C:109:LEU:HB2	1.98	0.44
1:B:160:PRO:C	1:B:277:MET:CE	2.85	0.44
1:C:80:ASP:OD2	1:C:82:ALA:HB3	2.18	0.44
1:C:230:LYS:NZ	3:C:692:HOH:O	2.50	0.44
1:B:175:LEU:CD2	1:B:232:THR:HG23	2.45	0.44
1:D:294:TYR:HB2	1:D:297:ILE:HD11	2.00	0.44
1:C:100:VAL:HG12	1:C:100:VAL:O	2.17	0.44
1:A:251:LYS:HD2	1:A:309:SER:O	2.18	0.44
1:B:18:LEU:C	1:B:18:LEU:HD23	2.38	0.44
1:A:287:THR:HG23	1:B:208:ASN:OD1	2.17	0.44
1:D:203:ARG:O	1:D:204:CYS:C	2.55	0.44
1:A:306:LEU:HG	1:A:307:ASN:OD1	2.18	0.44
1:A:298:PHE:HE1	1:A:313:LEU:HB3	1.82	0.43
1:A:230:LYS:HE3	3:A:650:HOH:O	2.18	0.43
1:D:333:TYR:CZ	1:D:337:ARG:HD2	2.53	0.43
1:B:242:ASP:O	1:B:243:VAL:HB	2.19	0.43
1:A:255:PRO:HB3	1:A:308:ASP:OD1	2.19	0.43
1:B:212:ALA:HB2	1:B:237:ARG:NH1	2.33	0.43
1:D:30:VAL:HG12	1:D:30:VAL:O	2.18	0.43
1:C:266:LYS:HG3	1:C:279:TYR:CZ	2.54	0.42
1:B:161:LEU:HA	1:B:277:MET:HE3	2.00	0.42
1:B:298:PHE:CZ	1:B:313:LEU:HD22	2.55	0.42
1:B:182:LEU:HD11	1:B:241:PRO:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASP:OD2	1:D:144:LYS:HE3	2.18	0.42
1:A:33:ASN:ND2	1:A:84:ILE:HD11	2.35	0.42
1:D:161:LEU:HA	1:D:277:MET:CE	2.49	0.42
1:B:160:PRO:CB	1:B:277:MET:HE1	2.46	0.42
1:B:80:ASP:OD2	1:B:83:GLU:HG2	2.20	0.42
1:B:30:VAL:O	1:B:30:VAL:HG12	2.18	0.42
1:D:298:PHE:HE1	1:D:313:LEU:HB3	1.84	0.42
1:A:200:ARG:NH1	3:A:463:HOH:O	2.53	0.42
1:A:297:ILE:HD12	1:A:297:ILE:N	2.34	0.42
1:C:200:ARG:HG2	1:D:283:ASP:HB3	2.02	0.41
1:B:298:PHE:HZ	1:B:313:LEU:HD22	1.85	0.41
1:D:298:PHE:CE1	1:D:303:CYS:SG	3.14	0.41
1:B:297:ILE:HD12	1:B:297:ILE:N	2.35	0.41
1:D:16:LEU:HD23	1:D:16:LEU:HA	1.88	0.41
1:C:78:ALA:HB3	1:C:84:ILE:HG12	2.02	0.41
1:A:92:GLN:HB3	1:A:339:LEU:HD13	2.03	0.41
1:D:46:LEU:HD12	3:D:732:HOH:O	2.21	0.41
1:A:269:SER:O	1:A:274:LYS:HA	2.21	0.41
1:B:41:TYR:CZ	1:C:192:PRO:HA	2.56	0.41
1:C:311:VAL:CG1	1:C:312:LYS:N	2.84	0.41
1:D:140:TYR:O	1:D:337:ARG:NH1	2.53	0.41
1:D:42:MET:HE2	1:D:66:LEU:HD11	2.01	0.41
1:A:141:ASP:HB3	1:A:144:LYS:HD2	2.02	0.41
1:A:161:LEU:HA	1:A:277:MET:CE	2.50	0.40
1:C:47:LYS:HG3	1:C:48:TYR:CE2	2.56	0.40
1:A:160:PRO:HB2	1:A:277:MET:HE1	2.03	0.40
1:A:65:ASP:OD1	1:A:74:LYS:HA	2.21	0.40
1:A:133:MET:O	1:A:276:ILE:HD13	2.21	0.40
1:A:200:ARG:NE	3:A:454:HOH:O	2.50	0.40
1:A:283:ASP:HB3	1:B:200:ARG:HG2	2.02	0.40
1:B:40:GLU:N	1:B:40:GLU:CD	2.72	0.40
1:C:255:PRO:HA	1:C:308:ASP:O	2.21	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	336/359 (94%)	321 (96%)	13 (4%)	2 (1%)	30	22
1	B	336/359 (94%)	321 (96%)	14 (4%)	1 (0%)	46	41
1	C	336/359 (94%)	320 (95%)	15 (4%)	1 (0%)	46	41
1	D	336/359 (94%)	325 (97%)	10 (3%)	1 (0%)	46	41
All	All	1344/1436 (94%)	1287 (96%)	52 (4%)	5 (0%)	39	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	VAL
1	C	243	VAL
1	D	243	VAL
1	A	198	ASP
1	B	243	VAL

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	276/294 (94%)	274 (99%)	2 (1%)	88	91
1	B	276/294 (94%)	274 (99%)	2 (1%)	88	91
1	C	276/294 (94%)	276 (100%)	0	100	100
1	D	276/294 (94%)	274 (99%)	2 (1%)	88	91
All	All	1104/1176 (94%)	1098 (100%)	6 (0%)	92	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	234	MET
1	B	234	MET
1	B	307	ASN
1	D	41	TYR
1	D	307	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
1	B	77	GLN
1	B	186	GLN
1	C	270	ASN
1	D	77	GLN
1	D	270	ASN
1	D	307	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	340	-	38,48,48	1.54	3 (7%)	47,73,73	2.17	9 (19%)
2	NAD	B	340	-	38,48,48	1.60	3 (7%)	47,73,73	2.13	8 (17%)
2	NAD	C	340	-	38,48,48	1.60	4 (10%)	47,73,73	2.12	7 (14%)
2	NAD	D	340	-	38,48,48	1.54	3 (7%)	47,73,73	2.19	8 (17%)

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	340	-	-	0/22/62/62	0/5/5/5
2	NAD	B	340	-	-	0/22/62/62	0/5/5/5
2	NAD	C	340	-	-	0/22/62/62	0/5/5/5
2	NAD	D	340	-	-	0/22/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	340	NAD	C4N-C3N	2.07	1.42	1.39
2	B	340	NAD	C2A-N1A	3.30	1.40	1.33
2	C	340	NAD	C2A-N1A	3.34	1.40	1.33
2	D	340	NAD	C2A-N1A	3.52	1.40	1.33
2	A	340	NAD	C2A-N1A	3.58	1.40	1.33
2	B	340	NAD	C2A-N3A	3.83	1.39	1.32
2	A	340	NAD	C2A-N3A	3.92	1.39	1.32
2	C	340	NAD	C2A-N3A	3.98	1.39	1.32
2	D	340	NAD	C2A-N3A	4.04	1.39	1.32
2	D	340	NAD	O7N-C7N	5.84	1.36	1.24
2	A	340	NAD	O7N-C7N	6.03	1.37	1.24
2	C	340	NAD	O7N-C7N	6.44	1.37	1.24
2	B	340	NAD	O7N-C7N	6.60	1.38	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	340	NAD	N3A-C2A-N1A	-11.08	120.41	128.89
2	D	340	NAD	N3A-C2A-N1A	-11.02	120.46	128.89
2	A	340	NAD	N3A-C2A-N1A	-10.98	120.48	128.89
2	C	340	NAD	N3A-C2A-N1A	-10.97	120.50	128.89
2	B	340	NAD	C4B-O4B-C1B	-4.40	104.88	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	340	NAD	C4B-O4B-C1B	-4.35	104.94	109.72
2	A	340	NAD	C4B-O4B-C1B	-4.02	105.30	109.72
2	D	340	NAD	C4B-O4B-C1B	-3.81	105.53	109.72
2	D	340	NAD	O7N-C7N-N7N	-3.19	118.10	122.59
2	C	340	NAD	C1B-N9A-C4A	-2.96	122.48	126.94
2	B	340	NAD	C1B-N9A-C4A	-2.95	122.49	126.94
2	B	340	NAD	O7N-C7N-N7N	-2.87	118.55	122.59
2	A	340	NAD	O7N-C7N-N7N	-2.86	118.57	122.59
2	C	340	NAD	O7N-C7N-N7N	-2.86	118.57	122.59
2	A	340	NAD	PN-O3-PA	-2.58	125.47	132.73
2	A	340	NAD	C1B-N9A-C4A	-2.41	123.30	126.94
2	D	340	NAD	PN-O3-PA	-2.39	126.02	132.73
2	C	340	NAD	C4A-C5A-N7A	-2.37	107.30	109.48
2	D	340	NAD	C1B-N9A-C4A	-2.29	123.49	126.94
2	B	340	NAD	C4A-C5A-N7A	-2.27	107.39	109.48
2	A	340	NAD	O7N-C7N-C3N	-2.23	117.15	119.59
2	D	340	NAD	O7N-C7N-C3N	-2.20	117.18	119.59
2	A	340	NAD	C4A-C5A-N7A	-2.19	107.47	109.48
2	B	340	NAD	PN-O3-PA	-2.06	126.94	132.73
2	D	340	NAD	C2B-C1B-N9A	2.50	118.11	114.29
2	B	340	NAD	C2B-C1B-N9A	2.66	118.35	114.29
2	A	340	NAD	C2B-C1B-N9A	2.77	118.53	114.29
2	C	340	NAD	C2B-C1B-N9A	2.85	118.65	114.29
2	B	340	NAD	C3N-C7N-N7N	5.13	123.43	117.82
2	C	340	NAD	C3N-C7N-N7N	5.13	123.43	117.82
2	A	340	NAD	C3N-C7N-N7N	5.91	124.28	117.82
2	D	340	NAD	C3N-C7N-N7N	6.30	124.72	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	340	NAD	1	0
2	C	340	NAD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	338/359 (94%)	0.02	5 (1%) 76 77	18, 30, 48, 56	0
1	B	338/359 (94%)	0.06	15 (4%) 38 39	17, 28, 51, 78	0
1	C	338/359 (94%)	0.34	27 (7%) 15 16	18, 34, 61, 82	0
1	D	338/359 (94%)	-0.01	7 (2%) 67 67	17, 27, 43, 57	0
All	All	1352/1436 (94%)	0.10	54 (3%) 42 44	17, 30, 51, 82	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	GLY	7.5
1	B	195	GLY	6.5
1	B	196	GLY	5.8
1	C	194	LYS	5.8
1	B	188	THR	5.4
1	B	194	LYS	5.3
1	D	339	LEU	4.4
1	C	189	VAL	4.4
1	B	189	VAL	4.4
1	B	193	SER	4.3
1	C	193	SER	4.0
1	C	339	LEU	3.9
1	C	2	THR	3.9
1	B	192	PRO	3.6
1	A	298	PHE	3.6
1	B	191	GLY	3.5
1	D	298	PHE	3.5
1	C	185	ASN	3.5
1	C	197	LYS	3.4
1	C	196	GLY	3.2
1	C	36	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	298	PHE	3.1
1	D	2	THR	3.1
1	B	186	GLN	3.0
1	D	197	LYS	3.0
1	C	192	PRO	3.0
1	C	116	LYS	2.9
1	A	339	LEU	2.7
1	C	337	ARG	2.7
1	B	183	THR	2.7
1	B	298	PHE	2.6
1	C	144	LYS	2.6
1	B	185	ASN	2.6
1	C	79	LYS	2.6
1	B	197	LYS	2.5
1	A	267	GLU	2.4
1	C	112	LYS	2.4
1	B	182	LEU	2.4
1	C	145	PHE	2.3
1	C	188	THR	2.3
1	C	101	PHE	2.3
1	C	83	GLU	2.3
1	D	38	ASP	2.2
1	A	307	ASN	2.2
1	B	187	LEU	2.2
1	C	142	PRO	2.2
1	D	127	ASN	2.2
1	C	108	SER	2.1
1	D	194	LYS	2.1
1	C	183	THR	2.1
1	A	195	GLY	2.1
1	C	187	LEU	2.0
1	C	143	SER	2.0
1	C	127	ASN	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 [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(\AA^2)	Q<0.9
2	NAD	B	340	44/44	0.88	0.18	1.01	40,48,54,54	0
2	NAD	C	340	44/44	0.88	0.16	0.24	42,48,53,54	0
2	NAD	A	340	44/44	0.95	0.11	-0.21	23,30,36,37	0
2	NAD	D	340	44/44	0.97	0.10	-0.39	16,24,26,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.