

Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 - 01:21 pm BST

PDB ID	:	8BR4
Title	:	Structure of GAPDH from Mycobacterium tuberculosis
Authors	:	Kumar, A.; Karthikeyan, S.
Deposited on	:	2022-11-22
Resolution	:	3.29 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.29 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.



Motrie	Whole archive	Similar resolution
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	357	83%	11%	5%
1	В	357	79%	16%	5%
1	С	357	83%	12%	5%
1	D	357	^{2%} 7 9%	16%	5%
1	Е	357	% 	16%	5%



Mol	Chain	Length	Quality of chain		
1	F	357	2% 82%	13%	5%
1	G	357	3% 82%	13%	5%
1	Н	357	82%	13%	5%
1	Ι	357	83%	12%	5%
1	J	357	82%	13%	5%
1	K	357	81%	13%	5%
1	L	357	81%	13%	5%
1	М	357	78%	17%	5%
1	Ν	357	79%	15%	5%
1	Ο	357	79%	16%	5%
1	Р	357	83%	12%	5%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 38389 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	330	Total	С	Ν	Ο	S	0	0	0
	Л	009	2363	1464	411	483	5	0	0	0
1	B	338	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	D	330	2364	1467	412	480	5	0	0	0
1	С	330	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
-	0	000	2344	1452	410	477	5	0	0	0
1	Д	338	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
			2347	1452	408	482	5	Ŭ		Ŭ
1	E	339	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
			2368	1468	411	484	5	Ŭ		
1	F	338	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	-		2370	1473	412	480	5	Ŭ		
1	G	339	Total	С	Ν	Ο	S	0	0	0
	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		2340	1448	409	478	5	Ŭ	Ŭ	
1	Н	338	Total	С	Ν	0	S	0	0	0
			2359	1459	411	484	5			
1	Ι	339	Total	C	N	0	S	0	0	0
			2366	1467	411	483	5		_	_
1	J	338	Total	C	N	0	S	0	0	0
			2371	1472	412	482	$\frac{5}{3}$			
1	К	339	Total	C	N	0	S	0	0	0
			2336	1446	408	477	5			
1	L	338	Total	C	N	0	S	0	0	0
			2344	1451	407	481	<u>5</u>			
1	М	339	Total	C	N	0	S	0	0	0
			2363	1464	411	483	<u>5</u>			
1	1 N	338	Total		N 410	100	S	0	0	0
			2364	1407	412	480	<u>5</u>			
1	0	339	Total	C	N 100	0	S	0	0	0
			2331	1441	408	4/7	5 C			
1	Р	338	Total	U 1450	IN 100	0	S	0	0	0
			2347	1452	408	482	5	_	-	

• Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.



Chain	Residue	Modelled	Actual	Comment	Reference
A	340	LEU	-	expression tag	UNP P9WN82
A	341	VAL	-	expression tag	UNP P9WN82
A	342	PRO	-	expression tag	UNP P9WN82
A	343	ARG	-	expression tag	UNP P9WN82
A	344	GLY	-	expression tag	UNP P9WN82
A	345	SER	-	expression tag	UNP P9WN82
А	346	GLY	-	expression tag	UNP P9WN82
А	347	GLY	-	expression tag	UNP P9WN82
А	348	GLY	-	expression tag	UNP P9WN82
А	349	GLY	-	expression tag	UNP P9WN82
А	350	HIS	-	expression tag	UNP P9WN82
А	351	HIS	-	expression tag	UNP P9WN82
А	352	HIS	-	expression tag	UNP P9WN82
А	353	HIS	-	expression tag	UNP P9WN82
А	354	HIS	-	expression tag	UNP P9WN82
А	355	HIS	-	expression tag	UNP P9WN82
А	356	HIS	-	expression tag	UNP P9WN82
А	357	HIS	-	expression tag	UNP P9WN82
В	340	LEU	-	expression tag	UNP P9WN82
В	341	VAL	-	expression tag	UNP P9WN82
В	342	PRO	-	expression tag	UNP P9WN82
В	343	ARG	-	expression tag	UNP P9WN82
В	344	GLY	-	expression tag	UNP P9WN82
В	345	SER	-	expression tag	UNP P9WN82
В	346	GLY	-	expression tag	UNP P9WN82
В	347	GLY	-	expression tag	UNP P9WN82
В	348	GLY	-	expression tag	UNP P9WN82
В	349	GLY	-	expression tag	UNP P9WN82
В	350	HIS	-	expression tag	UNP P9WN82
В	351	HIS	-	expression tag	UNP P9WN82
В	352	HIS	-	expression tag	UNP P9WN82
В	353	HIS	-	expression tag	UNP P9WN82
В	354	HIS	-	expression tag	UNP P9WN82
В	355	HIS	-	expression tag	UNP P9WN82
В	356	HIS	-	expression tag	UNP P9WN82
В	357	HIS	-	expression tag	UNP P9WN82
С	340	LEU	-	expression tag	UNP P9WN82
C	341	VAL	-	expression tag	UNP P9WN82
С	342	PRO	-	expression tag	UNP P9WN82
С	343	ARG	-	expression tag	UNP P9WN82
C	344	GLY	-	expression tag	UNP P9WN82
С	345	SER	-	expression tag	UNP P9WN82

There are 288 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
С	346	GLY	_	expression tag	UNP P9WN82
С	347	GLY	_	expression tag	UNP P9WN82
С	348	GLY	-	expression tag	UNP P9WN82
С	349	GLY	_	expression tag	UNP P9WN82
С	350	HIS	-	expression tag	UNP P9WN82
С	351	HIS	-	expression tag	UNP P9WN82
C	352	HIS	-	expression tag	UNP P9WN82
С	353	HIS	-	expression tag	UNP P9WN82
С	354	HIS	-	expression tag	UNP P9WN82
С	355	HIS	-	expression tag	UNP P9WN82
С	356	HIS	-	expression tag	UNP P9WN82
С	357	HIS	-	expression tag	UNP P9WN82
D	340	LEU	-	expression tag	UNP P9WN82
D	341	VAL	-	expression tag	UNP P9WN82
D	342	PRO	-	expression tag	UNP P9WN82
D	343	ARG	-	expression tag	UNP P9WN82
D	344	GLY	-	expression tag	UNP P9WN82
D	345	SER	-	expression tag	UNP P9WN82
D	346	GLY	-	expression tag	UNP P9WN82
D	347	GLY	-	expression tag	UNP P9WN82
D	348	GLY	-	expression tag	UNP P9WN82
D	349	GLY	-	expression tag	UNP P9WN82
D	350	HIS	-	expression tag	UNP P9WN82
D	351	HIS	-	expression tag	UNP P9WN82
D	352	HIS	-	expression tag	UNP P9WN82
D	353	HIS	-	expression tag	UNP P9WN82
D	354	HIS	-	expression tag	UNP P9WN82
D	355	HIS	-	expression tag	UNP P9WN82
D	356	HIS	-	expression tag	UNP P9WN82
D	357	HIS	-	expression tag	UNP P9WN82
E	340	LEU	-	expression tag	UNP P9WN82
E	341	VAL	-	expression tag	UNP P9WN82
E	342	PRO	-	expression tag	UNP P9WN82
E	343	ARG	-	expression tag	UNP P9WN82
E	344	GLY	-	expression tag	UNP P9WN82
E	345	SER	-	expression tag	UNP P9WN82
E	346	GLY	-	expression tag	UNP P9WN82
E	347	GLY	-	expression tag	UNP P9WN82
E	348	GLY	-	expression tag	UNP P9WN82
E	349	GLY	-	expression tag	UNP P9WN82
E	350	HIS	-	expression tag	UNP P9WN82
Е	351	HIS	-	expression tag	UNP P9WN82

Continued from previous page...



Chain	Residue	Modelled	Actual	Comment	Reference
Е	352	HIS	-	expression tag	UNP P9WN82
E	353	HIS	_	expression tag	UNP P9WN82
E	354	HIS	_	expression tag	UNP P9WN82
E	355	HIS	-	expression tag	UNP P9WN82
Е	356	HIS	-	expression tag	UNP P9WN82
Е	357	HIS	-	expression tag	UNP P9WN82
F	340	LEU	-	expression tag	UNP P9WN82
F	341	VAL	_	expression tag	UNP P9WN82
F	342	PRO	_	expression tag	UNP P9WN82
F	343	ARG	-	expression tag	UNP P9WN82
F	344	GLY	-	expression tag	UNP P9WN82
F	345	SER	-	expression tag	UNP P9WN82
F	346	GLY	-	expression tag	UNP P9WN82
F	347	GLY	-	expression tag	UNP P9WN82
F	348	GLY	-	expression tag	UNP P9WN82
F	349	GLY	-	expression tag	UNP P9WN82
F	350	HIS	-	expression tag	UNP P9WN82
F	351	HIS	-	expression tag	UNP P9WN82
F	352	HIS	-	expression tag	UNP P9WN82
F	353	HIS	-	expression tag	UNP P9WN82
F	354	HIS	-	expression tag	UNP P9WN82
F	355	HIS	-	expression tag	UNP P9WN82
F	356	HIS	-	expression tag	UNP P9WN82
F	357	HIS	-	expression tag	UNP P9WN82
G	340	LEU	-	expression tag	UNP P9WN82
G	341	VAL	-	expression tag	UNP P9WN82
G	342	PRO	-	expression tag	UNP P9WN82
G	343	ARG	-	expression tag	UNP P9WN82
G	344	GLY	-	expression tag	UNP P9WN82
G	345	SER	-	expression tag	UNP P9WN82
G	346	GLY	-	expression tag	UNP P9WN82
G	347	GLY	-	expression tag	UNP P9WN82
G	348	GLY	-	expression tag	UNP P9WN82
G	349	GLY	-	expression tag	UNP P9WN82
G	350	HIS	-	expression tag	UNP P9WN82
G	351	HIS	-	expression tag	UNP P9WN82
G	352	HIS	-	expression tag	UNP P9WN82
G	353	HIS	-	expression tag	UNP P9WN82
G	354	HIS	-	expression tag	UNP P9WN82
G	355	HIS	-	expression tag	UNP P9WN82
G	356	HIS	-	expression tag	UNP P9WN82
G	357	HIS	-	expression tag	UNP P9WN82



Chain	Residue	Modelled	Actual	Comment	Reference
Н	340	LEU	-	expression tag	UNP P9WN82
Н	341	VAL	-	expression tag	UNP P9WN82
Н	342	PRO	-	expression tag	UNP P9WN82
Н	343	ARG	-	expression tag	UNP P9WN82
Н	344	GLY	-	expression tag	UNP P9WN82
Н	345	SER	-	expression tag	UNP P9WN82
Н	346	GLY	-	expression tag	UNP P9WN82
Н	347	GLY	-	expression tag	UNP P9WN82
Н	348	GLY	-	expression tag	UNP P9WN82
Н	349	GLY	-	expression tag	UNP P9WN82
Н	350	HIS	-	expression tag	UNP P9WN82
Н	351	HIS	-	expression tag	UNP P9WN82
Н	352	HIS	-	expression tag	UNP P9WN82
Н	353	HIS	-	expression tag	UNP P9WN82
Н	354	HIS	-	expression tag	UNP P9WN82
Н	355	HIS	-	expression tag	UNP P9WN82
Н	356	HIS	-	expression tag	UNP P9WN82
Н	357	HIS	-	expression tag	UNP P9WN82
Ι	340	LEU	-	expression tag	UNP P9WN82
Ι	341	VAL	-	expression tag	UNP P9WN82
Ι	342	PRO	-	expression tag	UNP P9WN82
Ι	343	ARG	-	expression tag	UNP P9WN82
Ι	344	GLY	-	expression tag	UNP P9WN82
Ι	345	SER	-	expression tag	UNP P9WN82
Ι	346	GLY	-	expression tag	UNP P9WN82
Ι	347	GLY	-	expression tag	UNP P9WN82
Ι	348	GLY	-	expression tag	UNP P9WN82
Ι	349	GLY	-	expression tag	UNP P9WN82
Ι	350	HIS	-	expression tag	UNP P9WN82
Ι	351	HIS	-	expression tag	UNP P9WN82
Ι	352	HIS	-	expression tag	UNP P9WN82
Ι	353	HIS	-	expression tag	UNP P9WN82
Ι	354	HIS	-	expression tag	UNP P9WN82
Ι	355	HIS	-	expression tag	UNP P9WN82
Ι	356	HIS	-	expression tag	UNP P9WN82
Ι	357	HIS	-	expression tag	UNP P9WN82
J	340	LEU	-	expression tag	UNP P9WN82
J	341	VAL	-	expression tag	UNP P9WN82
J	342	PRO	-	expression tag	UNP P9WN82
J	343	ARG	-	expression tag	UNP P9WN82
J	344	GLY	-	expression tag	UNP P9WN82
J	345	SER	-	expression tag	UNP P9WN82



Chain	Residue	Modelled	Actual	Comment	Reference
J	346	GLY	-	expression tag	UNP P9WN82
J	347	GLY	-	expression tag	UNP P9WN82
J	348	GLY	-	expression tag	UNP P9WN82
J	349	GLY	-	expression tag	UNP P9WN82
J	350	HIS	-	expression tag	UNP P9WN82
J	351	HIS	-	expression tag	UNP P9WN82
J	352	HIS	-	expression tag	UNP P9WN82
J	353	HIS	-	expression tag	UNP P9WN82
J	354	HIS	-	expression tag	UNP P9WN82
J	355	HIS	-	expression tag	UNP P9WN82
J	356	HIS	-	expression tag	UNP P9WN82
J	357	HIS	-	expression tag	UNP P9WN82
K	340	LEU	-	expression tag	UNP P9WN82
K	341	VAL	-	expression tag	UNP P9WN82
K	342	PRO	-	expression tag	UNP P9WN82
K	343	ARG	-	expression tag	UNP P9WN82
K	344	GLY	-	expression tag	UNP P9WN82
K	345	SER	-	expression tag	UNP P9WN82
K	346	GLY	-	expression tag	UNP P9WN82
K	347	GLY	-	expression tag	UNP P9WN82
K	348	GLY	-	expression tag	UNP P9WN82
K	349	GLY	-	expression tag	UNP P9WN82
K	350	HIS	-	expression tag	UNP P9WN82
K	351	HIS	-	expression tag	UNP P9WN82
K	352	HIS	-	expression tag	UNP P9WN82
K	353	HIS	-	expression tag	UNP P9WN82
K	354	HIS	-	expression tag	UNP P9WN82
K	355	HIS	-	expression tag	UNP P9WN82
K	356	HIS	-	expression tag	UNP P9WN82
K	357	HIS	-	expression tag	UNP P9WN82
L	340	LEU	-	expression tag	UNP P9WN82
L	341	VAL	-	expression tag	UNP P9WN82
L	342	PRO	-	expression tag	UNP P9WN82
L	343	ARG	-	expression tag	UNP P9WN82
L	344	GLY	-	expression tag	UNP P9WN82
L	345	SER	-	expression tag	UNP P9WN82
L	346	GLY	-	expression tag	UNP P9WN82
L	347	GLY	-	expression tag	UNP P9WN82
L	348	GLY	-	expression tag	UNP P9WN82
L	349	GLY	-	expression tag	UNP P9WN82
L	350	HIS	-	expression tag	UNP P9WN82
L	351	HIS	-	expression tag	UNP P9WN82



Chain	Residue	Modelled	Actual	Comment	Reference
L	352	HIS	-	expression tag	UNP P9WN82
L	353	HIS	-	expression tag	UNP P9WN82
L	354	HIS	_	expression tag	UNP P9WN82
L	355	HIS	_	expression tag	UNP P9WN82
L	356	HIS	-	expression tag	UNP P9WN82
L	357	HIS	_	expression tag	UNP P9WN82
М	340	LEU	_	expression tag	UNP P9WN82
М	341	VAL	-	expression tag	UNP P9WN82
М	342	PRO	-	expression tag	UNP P9WN82
М	343	ARG	-	expression tag	UNP P9WN82
М	344	GLY	-	expression tag	UNP P9WN82
М	345	SER	-	expression tag	UNP P9WN82
М	346	GLY	-	expression tag	UNP P9WN82
М	347	GLY	-	expression tag	UNP P9WN82
М	348	GLY	-	expression tag	UNP P9WN82
М	349	GLY	-	expression tag	UNP P9WN82
М	350	HIS	-	expression tag	UNP P9WN82
М	351	HIS	-	expression tag	UNP P9WN82
М	352	HIS	_	expression tag	UNP P9WN82
М	353	HIS	-	expression tag	UNP P9WN82
М	354	HIS	-	expression tag	UNP P9WN82
М	355	HIS	-	expression tag	UNP P9WN82
М	356	HIS	-	expression tag	UNP P9WN82
М	357	HIS	-	expression tag	UNP P9WN82
N	340	LEU	-	expression tag	UNP P9WN82
N	341	VAL	-	expression tag	UNP P9WN82
N	342	PRO	-	expression tag	UNP P9WN82
N	343	ARG	-	expression tag	UNP P9WN82
N	344	GLY	-	expression tag	UNP P9WN82
N	345	SER	-	expression tag	UNP P9WN82
N	346	GLY	-	expression tag	UNP P9WN82
N	347	GLY	-	expression tag	UNP P9WN82
N	348	GLY	-	expression tag	UNP P9WN82
N	349	GLY	-	expression tag	UNP P9WN82
N	350	HIS	-	expression tag	UNP P9WN82
N	351	HIS	-	expression tag	UNP P9WN82
Ν	352	HIS	-	expression tag	UNP P9WN82
N	353	HIS	-	expression tag	UNP P9WN82
N	354	HIS	-	expression tag	UNP P9WN82
N	355	HIS	-	expression tag	UNP P9WN82
N	356	HIS	-	expression tag	UNP P9WN82
N	357	HIS	-	expression tag	UNP P9WN82



Chain	Residue	Modelled	Actual	Comment	Reference
0	340	LEU	-	expression tag	UNP P9WN82
0	341	VAL	-	expression tag	UNP P9WN82
0	342	PRO	-	expression tag	UNP P9WN82
0	343	ARG	-	expression tag	UNP P9WN82
0	344	GLY	-	expression tag	UNP P9WN82
0	345	SER	-	expression tag	UNP P9WN82
0	346	GLY	-	expression tag	UNP P9WN82
0	347	GLY	-	expression tag	UNP P9WN82
0	348	GLY	-	expression tag	UNP P9WN82
0	349	GLY	-	expression tag	UNP P9WN82
0	350	HIS	-	expression tag	UNP P9WN82
0	351	HIS	-	expression tag	UNP P9WN82
0	352	HIS	-	expression tag	UNP P9WN82
0	353	HIS	-	expression tag	UNP P9WN82
0	354	HIS	-	expression tag	UNP P9WN82
0	355	HIS	-	expression tag	UNP P9WN82
0	356	HIS	-	expression tag	UNP P9WN82
0	357	HIS	-	expression tag	UNP P9WN82
P	340	LEU	-	expression tag	UNP P9WN82
P	341	VAL	-	expression tag	UNP P9WN82
P	342	PRO	-	expression tag	UNP P9WN82
P	343	ARG	-	expression tag	UNP P9WN82
P	344	GLY	-	expression tag	UNP P9WN82
P	345	SER	-	expression tag	UNP P9WN82
P	346	GLY	-	expression tag	UNP P9WN82
P	347	GLY	-	expression tag	UNP P9WN82
P	348	GLY	-	expression tag	UNP P9WN82
P	349	GLY	-	expression tag	UNP P9WN82
P	350	HIS	-	expression tag	UNP P9WN82
P	351	HIS	-	expression tag	UNP P9WN82
P	352	HIS	-	expression tag	UNP P9WN82
P	353	HIS	-	expression tag	UNP P9WN82
P	354	HIS	-	expression tag	UNP P9WN82
P	355	HIS	-	expression tag	UNP P9WN82
P	356	HIS	-	expression tag	UNP P9WN82
P	357	HIS	-	expression tag	UNP P9WN82

• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).





$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2       A       1       44       21       7       14       2       0       0         2       B       1       Total       C       N       O       P       0       0         2       B       1       Total       C       N       O       P       0       0         2       C       1       Total       C       N       O       P       0       0         2       D       1       Total       C       N       O       P       0       0         2       D       1       Total       C       N       O       P       0       0         2       D       1       Total       C       N       O       P       0       0         2       F       1       Total       C       N       O       P       0       0         2       F       1       Total       C       N       O       P       0       0         2       G       1       Total       C       N       O       P       0       0         2       H       1       Total       C	0	٨	1	Total	С	Ν	Ο	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	А	1	44	21	$\overline{7}$	14	2	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0	D	1	Total	С	Ν	Ο	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		D	1	44	21	7	14	2	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	С	1	Total	С	Ν	Ο	Р	0	Ο
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	U	1	44	21	$\overline{7}$	14	2	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	Л	1	Total	С	Ν	Ο	Р	0	Ο
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		D	I	44	21	7	14	2	0	0
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	2	E	1	Total	$\mathbf{C}$	Ν	Ο	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			1	44	21	7	14	2	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	F	1	Total	С	Ν	Ο	Р	Ο	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	1	44	21	7	14	2	0	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	G	1	Total	С	Ν	Ο	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		5	-	44	21	7	14	2	0	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	Н	1	Total	С	Ν	0	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			_	44	21	7	14	2		-
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	Ι	1	Total	C	N	0	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				44	21	<u>'7</u>	14	2		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	J	1	Total	C	N	0	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				44	21	<u>'</u> /	14	2		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	Κ	1	Total	C	N	0	Р	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				44	21	7 	14	2		
44         21         7         14         2           Total         C         N         O         P         0         0	2	L	1	Total	C	N	0	Р	0	0
I I I I I I I I I I I I I I I I I I I				44	21		14	2		
	2	М	1	Total	C 01	IN 7		P	0	0
				44	21	( 	14	2		
$\begin{vmatrix} 2 \\ N \end{vmatrix}$ $\begin{vmatrix} 1 \\ 44 \\ 21 \\ 7 \\ 14 \\ 2 \end{vmatrix}$ $\begin{vmatrix} 0 \\ 0 \\ 0 \end{vmatrix}$ $\begin{vmatrix} 0 \\ 0 \\ 0 \end{vmatrix}$	2	Ν	1		U 91	IN 7	14	Р о	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	0	1	Total	С	Ν	Ο	Р	0	0
	1	44	21	7	14	2	0	0	
0	D	1	Total	С	Ν	Ο	Р	0	0
2 P		44	21	7	14	2	0	0	

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 4  2  2 \end{array}$	0	0



Chain D:

### 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



16%

5%

79%

# SER GLY GLY GLY GLY HIS HIS HIS HIS HIS HIS HIS HIS • Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Chain E: 79% 5% 16% VAL PRO GLY GLY GLY GLY GLY HIS HIS SIH SIH SIH SIH • Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Chain F: 82% 13% 5% LEU VAL PRO ARG GLY SER • Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Chain G: 82% 13% 5% • Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Chain H: 82% 13% 5%









• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	140.89Å 139.17Å 141.48Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $108.52^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	47.15 - 3.29	Depositor
Resolution (A)	48.29 - 3.29	EDS
% Data completeness	99.2 (47.15-3.29)	Depositor
(in resolution range)	99.3 (48.29-3.29)	EDS
R _{merge}	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.39 (at 3.25 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.255 , $0.295$	Depositor
$n, n_{free}$	0.253 , $0.293$	DCC
$R_{free}$ test set	3965 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	63.3	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, $63.9$	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	38389	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.13% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

## 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: EDO, 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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.24	0/2400	0.45	0/3289	
1	В	0.24	0/2401	0.46	0/3290	
1	С	0.24	0/2381	0.45	0/3263	
1	D	0.24	0/2384	0.46	0/3268	
1	Е	0.24	0/2405	0.46	0/3296	
1	F	0.24	0/2407	0.45	0/3298	
1	G	0.24	0/2377	0.45	0/3260	
1	Н	0.24	0/2396	0.46	0/3283	
1	Ι	0.24	0/2403	0.45	0/3293	
1	J	0.24	0/2408	0.46	0/3299	
1	Κ	0.24	0/2373	0.46	0/3255	
1	L	0.24	0/2381	0.45	0/3264	
1	М	0.24	0/2400	0.45	0/3289	
1	Ν	0.24	0/2401	0.46	0/3290	
1	0	0.24	0/2368	0.45	0/3248	
1	Р	0.24	0/2384	0.45	0/3268	
All	All	0.24	0/38269	0.45	0/52453	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (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.



8BR4
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2363	0	2133	31	0
1	В	2364	0	2156	40	0
1	С	2344	0	2105	27	0
1	D	2347	0	2101	40	0
1	Е	2368	0	2147	40	0
1	F	2370	0	2174	34	0
1	G	2340	0	2089	29	0
1	Н	2359	0	2123	37	0
1	Ι	2366	0	2142	35	0
1	J	2371	0	2169	35	0
1	K	2336	0	2083	37	0
1	L	2344	0	2097	37	0
1	М	2363	0	2133	44	0
1	N	2364	0	2156	37	0
1	0	2331	0	2067	41	0
1	Р	2347	0	2101	37	0
2	А	44	0	26	4	0
2	В	44	0	26	2	0
2	С	44	0	26	1	0
2	D	44	0	26	3	0
2	Е	44	0	26	3	0
2	F	44	0	26	1	0
2	G	44	0	26	0	0
2	Н	44	0	26	0	0
2	Ι	44	0	26	5	0
2	J	44	0	26	2	0
2	Κ	44	0	26	2	0
2	L	44	0	26	2	0
2	М	44	0	26	2	0
2	N	44	0	26	1	0
2	0	44	0	26	2	0
2	Р	44	0	26	2	0
3	A	4	0	6	0	0
3	D	4	0	6	0	0
All	All	38389	0	34404	480	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 7.

All (480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:N:209:LEU:HD21	1:P:243:PRO:HG3	1.57	0.86
1:H:291:ILE:HG23	1:H:299:ILE:HD12	1.70	0.73
1:I:291:ILE:HG23	1:I:299:ILE:HD12	1.72	0.71
1:E:290:ASP:OD1	1:H:205:ARG:NH2	2.24	0.71
1:0:185:HIS:HB3	1:O:239:ARG:HD3	1.73	0.70
1:J:310:ASP:OD1	1:K:178:LYS:NZ	2.23	0.67
1:D:38:ASN:HA	1:D:81:LEU:HA	1.75	0.66
1:E:243:PRO:O	1:E:244:THR:HG22	1.94	0.66
1:N:290:ASP:OD1	1:O:205:ARG:NH2	2.28	0.66
1:B:290:ASP:OD1	1:C:205:ARG:NH2	2.28	0.66
1:F:299:ILE:HB	1:F:317:TRP:HB2	1.78	0.65
1:L:291:ILE:HG23	1:L:299:ILE:HD12	1.78	0.65
1:G:297:SER:HG	1:G:327:ARG:HH11	1.41	0.65
1:B:298:SER:HG	1:B:316:SER:HG	1.45	0.64
1:A:290:ASP:OD1	1:D:205:ARG:NH2	2.30	0.64
1:O:211:ILE:HG22	1:O:240:VAL:HA	1.78	0.64
1:J:222:ILE:HG21	1:J:233:LEU:HD12	1.79	0.64
1:E:182:THR:OG1	1:H:313:LYS:NZ	2.27	0.63
1:P:25:GLN:NE2	1:P:32:VAL:O	2.31	0.63
1:E:58:ARG:NH2	1:F:292:VAL:O	2.32	0.63
1:M:291:ILE:HG23	1:M:299:ILE:HD12	1.79	0.63
1:N:55:ILE:HD13	1:N:244:THR:HG23	1.80	0.63
1:D:291:ILE:HG23	1:D:299:ILE:HD12	1.80	0.62
1:L:185:HIS:HB3	1:L:239:ARG:HD3	1.81	0.62
1:I:182:THR:OG1	1:L:313:LYS:NZ	2.27	0.61
1:E:185:HIS:HB3	1:E:239:ARG:HD3	1.83	0.61
1:K:185:HIS:HB3	1:K:239:ARG:HD3	1.81	0.61
1:M:182:THR:OG1	1:P:313:LYS:NZ	2.29	0.61
1:J:260:VAL:HG23	1:J:307:VAL:HG12	1.81	0.61
1:I:185:HIS:HB3	1:I:239:ARG:HD3	1.83	0.60
1:O:12:ARG:HH11	1:O:15:ARG:HH21	1.49	0.60
1:J:290:ASP:OD1	1:K:205:ARG:NH2	2.28	0.60
1:O:292:VAL:O	1:P:58:ARG:NH2	2.33	0.60
1:I:54:SER:HA	1:J:289:SER:HB3	1.84	0.60
1:L:139:LEU:HD12	1:L:327:ARG:HD3	1.84	0.60
1:I:286:ILE:O	1:L:202:ARG:NH1	2.35	0.60
1:J:205:ARG:NH2	1:K:290:ASP:OD1	2.35	0.60
1:L:10:PHE:N	1:L:39:ASP:OD1	2.35	0.60
1:G:291:ILE:HG23	1:G:299:ILE:HD12	1.82	0.59
1:O:297:SER:OG	1:O:327:ARG:NH1	2.28	0.59
1:D:185:HIS:HB3	1:D:239:ARG:HD3	1.83	0.59
1:E:54:SER:OG	1:G:205:ARG:NH1	2.36	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:202:ARG:NH1	1:D:286:ILE:O	2.35	0.59
1:G:10:PHE:N	1:G:39:ASP:OD1	2.36	0.59
1:F:320:ASN:HD22	2:F:401:NAD:H72N	1.50	0.59
1:H:185:HIS:HB3	1:H:239:ARG:HD3	1.84	0.58
1:C:185:HIS:HB3	1:C:239:ARG:HD3	1.85	0.58
1:D:135:ILE:HG23	1:D:153:ILE:HG23	1.86	0.58
1:O:12:ARG:N	2:O:401:NAD:O2N	2.37	0.58
1:M:8:ASN:ND2	1:M:102:GLU:OE1	2.36	0.58
1:M:178:LYS:NZ	1:P:310:ASP:OD1	2.32	0.58
1:A:12:ARG:HH11	1:A:15:ARG:HH21	1.51	0.58
1:A:291:ILE:HG23	1:A:299:ILE:HD12	1.86	0.58
1:N:202:ARG:HD2	1:N:213:PRO:HG2	1.86	0.58
1:C:291:ILE:HG23	1:C:299:ILE:HD12	1.84	0.57
1:K:289:SER:HB3	1:L:54:SER:HA	1.85	0.57
1:F:209:LEU:HD11	1:H:243:PRO:HB3	1.87	0.57
1:J:202:ARG:HD2	1:J:213:PRO:HG2	1.86	0.57
1:O:260:VAL:HG23	1:O:307:VAL:HG12	1.87	0.57
1:G:297:SER:OG	1:G:327:ARG:NH1	2.32	0.57
1:I:54:SER:OG	1:K:205:ARG:NH1	2.36	0.57
1:E:222:ILE:HG21	1:E:233:LEU:HD12	1.87	0.57
1:J:185:HIS:HB3	1:J:239:ARG:HD3	1.87	0.57
1:B:194:GLN:HE22	1:D:55:ILE:HD11	1.69	0.57
1:M:195:ASP:O	1:O:15:ARG:NH2	2.30	0.57
1:N:15:ARG:NH2	1:P:195:ASP:O	2.35	0.57
1:J:320:ASN:HD22	2:J:401:NAD:H72N	1.52	0.56
1:M:39:ASP:OD1	2:M:401:NAD:H1B	2.04	0.56
1:P:291:ILE:HG23	1:P:299:ILE:HD12	1.87	0.56
1:E:138:VAL:HG23	1:E:225:VAL:HG11	1.86	0.56
1:K:39:ASP:OD2	2:K:401:NAD:O3B	2.22	0.56
1:N:194:GLN:HE22	1:P:55:ILE:HD11	1.69	0.56
1:O:291:ILE:HG23	1:O:299:ILE:HD12	1.86	0.56
1:C:195:ASP:OD2	1:C:205:ARG:NH1	2.39	0.56
1:J:195:ASP:O	1:L:15:ARG:NH2	2.33	0.56
1:M:25:GLN:NE2	1:M:32:VAL:O	2.39	0.56
1:O:181:MET:HG3	1:O:235:GLY:HA3	1.87	0.56
1:L:322:TRP:O	1:L:326:ASN:ND2	2.35	0.56
1:M:188:THR:OG1	1:M:190:ASP:OD1	2.21	0.56
1:A:211:ILE:HG22	1:A:240:VAL:HA	1.87	0.56
1:C:12:ARG:HH11	1:C:15:ARG:HH21	1.54	0.56
1:K:39:ASP:OD1	1:K:40:ILE:N	2.36	0.56
1:L:202:ARG:HD2	1:L:213:PRO:HG2	1.88	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:138:VAL:HG23	1:I:225:VAL:HG11	1.87	0.56
1:J:209:LEU:HD11	1:L:243:PRO:HB3	1.86	0.56
1:I:39:ASP:OD1	1:I:40:ILE:N	2.39	0.55
1:J:286:ILE:O	1:K:202:ARG:NH1	2.39	0.55
1:M:286:ILE:O	1:P:202:ARG:NH1	2.38	0.55
1:F:185:HIS:HB3	1:F:239:ARG:HD3	1.87	0.55
1:F:55:ILE:HD13	1:F:244:THR:HG23	1.88	0.55
1:B:138:VAL:HG23	1:B:225:VAL:HG11	1.89	0.55
1:P:202:ARG:HD2	1:P:213:PRO:HG2	1.89	0.55
1:N:185:HIS:HB3	1:N:239:ARG:HD3	1.89	0.55
1:C:190:ASP:OD2	1:C:203:ARG:NH1	2.40	0.55
1:L:299:ILE:HB	1:L:317:TRP:HB2	1.88	0.55
1:B:291:ILE:HG23	1:B:299:ILE:HD12	1.89	0.54
1:N:4:ARG:NH1	1:N:95:LEU:O	2.41	0.54
1:F:194:GLN:HE22	1:H:55:ILE:HD11	1.72	0.54
1:N:180:LEU:HD21	1:O:308:ILE:HG13	1.88	0.54
1:M:211:ILE:HG22	1:M:240:VAL:HA	1.90	0.54
1:O:138:VAL:HG23	1:O:225:VAL:HG11	1.89	0.54
1:B:54:SER:OG	1:D:205:ARG:NH1	2.41	0.54
1:C:138:VAL:HG23	1:C:225:VAL:HG11	1.89	0.54
1:H:211:ILE:HG22	1:H:240:VAL:HA	1.88	0.54
1:J:202:ARG:NH1	1:K:286:ILE:O	2.38	0.54
1:K:211:ILE:HG22	1:K:240:VAL:HA	1.89	0.53
1:M:213:PRO:HD2	1:P:287:VAL:HG12	1.90	0.53
1:O:170:LEU:HD11	1:O:314:VAL:HG21	1.90	0.53
1:P:188:THR:OG1	1:P:190:ASP:OD1	2.19	0.53
1:B:39:ASP:OD1	2:B:401:NAD:H1B	2.08	0.53
1:J:205:ARG:NH1	1:L:54:SER:OG	2.41	0.53
1:K:170:LEU:HD13	1:K:252:VAL:HG11	1.91	0.53
1:L:12:ARG:HH11	1:L:15:ARG:HH21	1.56	0.53
1:0:188:THR:OG1	1:0:190:ASP:OD1	2.22	0.53
1:L:211:ILE:HG22	1:L:240:VAL:HA	1.90	0.53
1:M:185:HIS:HB3	1:M:239:ARG:HD3	1.90	0.53
1:O:322:TRP:O	1:O:326:ASN:ND2	2.37	0.53
1:J:15:ARG:NH2	1:L:195:ASP:O	2.37	0.53
1:G:12:ARG:HH11	1:G:15:ARG:HH21	1.57	0.53
1:I:180:LEU:HB3	1:L:313:LYS:HE3	1.91	0.52
1:J:190:ASP:OD2	1:J:203:ARG:NH1	2.42	0.52
1:B:205:ARG:NH1	1:D:54:SER:OG	2.43	0.52
1:E:180:LEU:HB3	1:H:313:LYS:HE3	1.91	0.52
1:F:205:ARG:NH2	1:G:290:ASP:OD1	2.42	0.52



	lo uo puge	Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap(Å)	
1:M:9:GLY:HA2	2:M:401:NAD:H8A	1.91	0.52	
1:F:188:THR:OG1	1:F:190:ASP:OD1	2.23	0.52	
1:A:213:PRO:HD2	1:D:287:VAL:HG12	1.91	0.52	
1:G:185:HIS:HB3	1:G:239:ARG:HD3	1.91	0.51	
1:I:39:ASP:HA	2:I:401:NAD:C8A	2.41	0.51	
1:K:141:VAL:HG21	1:K:164:ALA:HB1	1.92	0.51	
1:P:39:ASP:HA	2:P:401:NAD:H8A	1.91	0.51	
1:E:15:ARG:NH2	1:G:195:ASP:O	2.37	0.51	
1:E:202:ARG:HD2	1:E:213:PRO:HG2	1.91	0.51	
1:H:299:ILE:HB	1:H:317:TRP:HB2	1.92	0.51	
1:M:180:LEU:HB3	1:P:313:LYS:HE3	1.92	0.51	
1:A:202:ARG:HD2	1:A:213:PRO:HG2	1.91	0.51	
1:O:202:ARG:HD2	1:0:213:PRO:HG2	1.92	0.51	
1:F:260:VAL:HG23	1:F:307:VAL:HG12	1.92	0.51	
1:G:202:ARG:HD3	1:G:213:PRO:HG2	1.92	0.51	
1:O:69:ASP:HA	1:O:79:LYS:H	1.76	0.51	
1:B:4:ARG:NH1	1:B:95:LEU:O	2.44	0.51	
1:B:211:ILE:HG22	1:B:240:VAL:HA	1.91	0.51	
1:B:322:TRP:O	1:B:326:ASN:ND2	2.34	0.51	
1:H:195:ASP:OD2	1:H:205:ARG:NH1	2.44	0.51	
1:J:53:ASP:C	1:L:205:ARG:HH22	2.14	0.51	
1:A:39:ASP:HA	2:A:401:NAD:C8A	2.40	0.51	
1:B:202:ARG:NH1	1:C:286:ILE:O	2.42	0.51	
1:K:288:SER:O	1:K:291:ILE:HG22	2.11	0.51	
1:I:139:LEU:HD12	1:I:327:ARG:HD3	1.93	0.51	
1:A:54:SER:HA	1:B:289:SER:HB3	1.93	0.51	
1:F:190:ASP:OD2	1:F:203:ARG:NH1	2.44	0.51	
1:D:202:ARG:HD2	1:D:213:PRO:HG2	1.93	0.50	
1:E:25:GLN:NE2	1:E:32:VAL:O	2.44	0.50	
1:I:166:LEU:HD11	1:I:316:SER:HB3	1.93	0.50	
1:K:163:LEU:HD11	1:K:250:LEU:HD22	1.92	0.50	
1:M:260:VAL:HG23	1:M:307:VAL:HG12	1.94	0.50	
1:A:166:LEU:HD11	1:A:316:SER:HB3	1.94	0.50	
1:N:205:ARG:NH1	1:P:54:SER:OG	2.44	0.50	
1:A:138:VAL:HG23	1:A:225:VAL:HG11	1.93	0.50	
1:B:286:ILE:O	1:C:202:ARG:NH1	2.44	0.50	
1:G:170:LEU:HD13	1:G:252:VAL:HG11	1.93	0.50	
1:I:195:ASP:O	1:K:15:ARG:NH2	2.36	0.50	
1:G:54:SER:HA	1:H:289:SER:HB3	1.93	0.50	
1:J:291:ILE:HD11	1:J:299:ILE:HG21	1.93	0.50	
1:E:260:VAL:HG23	1:E:307:VAL:HG12	1.94	0.50	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:M:9:GLY:O	1:M:103:SER:OG	2.30	0.50	
1:E:180:LEU:HD21	1:H:308:ILE:HG12	1.94	0.50	
1:O:299:ILE:HB	1:O:317:TRP:HB2	1.94	0.50	
1:A:185:HIS:HB3	1:A:239:ARG:HD3	1.94	0.50	
1:I:12:ARG:HH11	1:I:15:ARG:HH21	1.58	0.50	
1:M:12:ARG:HH11	1:M:15:ARG:HH21	1.58	0.50	
1:E:91:PRO:HB2	1:E:94:ASP:HB2	1.94	0.50	
1:F:298:SER:OG	1:F:316:SER:OG	2.22	0.50	
1:N:209:LEU:CD2	1:P:243:PRO:HG3	2.36	0.50	
1:B:15:ARG:NH2	1:D:195:ASP:O	2.38	0.49	
1:F:298:SER:HG	1:F:316:SER:HG	1.51	0.49	
1:N:51:LYS:NZ	1:N:59:LEU:O	2.36	0.49	
1:E:286:ILE:O	1:H:202:ARG:NH1	2.42	0.49	
1:G:292:VAL:O	1:H:58:ARG:NH2	2.44	0.49	
1:P:322:TRP:O	1:P:326:ASN:ND2	2.38	0.49	
1:D:10:PHE:N	1:D:39:ASP:OD1	2.46	0.49	
1:A:12:ARG:HB2	2:A:401:NAD:O1N	2.13	0.49	
1:A:180:LEU:HB3	1:D:313:LYS:HE2	1.93	0.49	
1:B:320:ASN:HD22	2:B:401:NAD:H72N	1.61	0.49	
1:G:141:VAL:HG21	1:G:164:ALA:HB1	1.93	0.49	
1:M:170:LEU:HD13	1:M:252:VAL:HG11	1.94	0.49	
1:G:138:VAL:HG23	1:G:225:VAL:HG11	1.93	0.49	
1:M:202:ARG:HD2	1:M:213:PRO:HG2	1.94	0.49	
1:K:291:ILE:HD11	1:K:299:ILE:HD12	1.95	0.49	
1:L:267:PHE:HD1	1:L:279:LEU:HD21	1.77	0.49	
1:M:138:VAL:HG23	1:M:225:VAL:HG11	1.93	0.49	
1:N:297:SER:OG	1:N:327:ARG:NH1	2.34	0.49	
1:B:12:ARG:HH11	1:B:15:ARG:HH21	1.59	0.49	
1:D:211:ILE:HG22	1:D:240:VAL:HA	1.95	0.49	
1:J:178:LYS:NZ	1:J:253:ASP:OD2	2.46	0.49	
1:D:271:ALA:HB2	1:D:279:LEU:HD22	1.94	0.48	
1:J:180:LEU:HB3	1:K:313:LYS:HE2	1.94	0.48	
1:P:39:ASP:HA	2:P:401:NAD:C8A	2.43	0.48	
1:J:8:ASN:ND2	1:J:102:GLU:OE1	2.43	0.48	
1:N:138:VAL:HG23	1:N:225:VAL:HG11	1.95	0.48	
1:M:110:ALA:HA	1:M:113:ALA:HB3	1.94	0.48	
1:D:299:ILE:HB	1:D:317:TRP:HB2	1.96	0.48	
1:O:11:GLY:HA3	2:O:401:NAD:O5B	2.13	0.48	
1:B:8:ASN:ND2	1:B:102:GLU:OE1	2.45	0.48	
1:F:138:VAL:HG23	1:F:225:VAL:HG11	1.95	0.48	
1:L:51:LYS:HD2	1:L:59:LEU:HB3	1.94	0.48	



	to ac pagem	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
1:A:19:ARG:NH2	1:A:50:LEU:O	2.47	0.48	
1:A:39:ASP:HA	2:A:401:NAD:H8A	1.96	0.48	
1:G:4:ARG:NH1	1:G:95:LEU:O	2.47	0.48	
1:G:163:LEU:HD22	1:G:181:MET:SD	2.54	0.48	
1:K:162:CYS:HA	1:K:298:SER:HB2	1.95	0.48	
1:K:138:VAL:HG23	1:K:225:VAL:HG11	1.96	0.47	
1:L:163:LEU:HD22	1:L:181:MET:SD	2.54	0.47	
1:N:280:LYS:HB2	1:N:296:HIS:CD2	2.48	0.47	
1:P:138:VAL:HG23	1:P:225:VAL:HG11	1.96	0.47	
1:E:247:VAL:HB	1:E:317:TRP:CE3	2.49	0.47	
1:H:257:ARG:HH21	1:N:231:GLY:HA3	1.80	0.47	
1:N:170:LEU:HD11	1:N:314:VAL:HG21	1.96	0.47	
1:N:188:THR:OG1	1:N:239:ARG:NH1	2.48	0.47	
1:G:191:GLN:OE1	1:G:239:ARG:NH1	2.46	0.47	
1:I:39:ASP:HA	2:I:401:NAD:H8A	1.97	0.47	
1:J:317:TRP:HZ2	1:K:213:PRO:HG3	1.80	0.47	
1:D:138:VAL:HG23	1:D:225:VAL:HG11	1.97	0.47	
1:J:12:ARG:HH11	1:J:15:ARG:HH21	1.62	0.47	
1:K:139:LEU:HA	1:K:143:ASP:HB3	1.97	0.47	
1:M:166:LEU:HD11	1:M:316:SER:HB3	1.96	0.47	
1:M:222:ILE:HG21	1:M:233:LEU:HD12	1.95	0.47	
1:B:202:ARG:HD2	1:B:213:PRO:HG2	1.95	0.47	
1:H:322:TRP:O	1:H:326:ASN:ND2	2.42	0.47	
1:D:190:ASP:O	1:D:198:HIS:NE2	2.38	0.47	
1:E:100:VAL:HG11	1:E:116:HIS:ND1	2.29	0.47	
1:E:211:ILE:HG23	1:H:242:ILE:HD11	1.96	0.47	
1:K:38:ASN:ND2	2:K:401:NAD:H2A	2.30	0.47	
1:P:17:PHE:HA	1:P:325:SER:HB3	1.97	0.47	
1:A:54:SER:N	1:C:205:ARG:HH12	2.13	0.47	
1:B:185:HIS:HB3	1:B:239:ARG:HD3	1.96	0.47	
1:B:195:ASP:O	1:D:15:ARG:NH2	2.39	0.47	
1:E:166:LEU:HD11	1:E:316:SER:HB3	1.97	0.47	
1:E:240:VAL:O	1:E:242:ILE:N	2.48	0.47	
1:G:267:PHE:HD1	1:G:279:LEU:HD21	1.80	0.46	
1:A:144:ASP:OD1	1:A:144:ASP:N	2.47	0.46	
1:E:12:ARG:NH2	1:E:321:GLU:OE1	2.45	0.46	
1:F:12:ARG:HH11	1:F:15:ARG:HH21	1.64	0.46	
1:0:190:ASP:0	1:O:198:HIS:NE2	2.45	0.46	
1:B:299:ILE:HB	1:B:317:TRP:HB2	1.97	0.46	
1:D:163:LEU:HD11	1:D:250:LEU:HD22	1.97	0.46	
1:N:12:ARG:HH11	1:N:15:ARG:HH21	1.64	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:P:185:HIS:HB3	1:P:239:ARG:HD3	1.98	0.46	
1:C:163:LEU:HD22	1:C:181:MET:SD	2.56	0.46	
1:F:201:LEU:HB3	1:H:48:HIS:CE1	2.50	0.46	
1:L:298:SER:OG	1:L:316:SER:OG	2.22	0.46	
1:P:248:THR:HG23	1:P:318:TYR:CE1	2.50	0.46	
1:H:138:VAL:HG23	1:H:225:VAL:HG11	1.97	0.46	
1:J:100:VAL:HG11	1:J:116:HIS:ND1	2.30	0.46	
1:O:163:LEU:HD11	1:O:250:LEU:HD22	1.97	0.46	
1:D:161:ASN:O	1:D:297:SER:OG	2.26	0.46	
1:L:170:LEU:HD13	1:L:252:VAL:HG11	1.98	0.46	
1:C:188:THR:OG1	1:C:239:ARG:NH1	2.46	0.46	
1:G:15:ARG:HD2	1:G:50:LEU:HA	1.98	0.46	
1:M:202:ARG:NH1	1:P:286:ILE:O	2.47	0.46	
1:N:322:TRP:O	1:N:326:ASN:ND2	2.39	0.46	
1:N:3:VAL:HG21	1:N:336:GLY:HA3	1.98	0.46	
1:O:92:TRP:HD1	1:O:119:ALA:HB3	1.81	0.46	
1:E:39:ASP:HA	2:E:401:NAD:C8A	2.46	0.45	
1:E:188:THR:OG1	1:E:239:ARG:NH1	2.48	0.45	
1:H:271:ALA:HB2	1:H:279:LEU:HD22	1.98	0.45	
1:N:291:ILE:HD12	1:N:299:ILE:HD12	1.98	0.45	
1:E:211:ILE:HG22	1:E:240:VAL:HA	1.99	0.45	
1:I:185:HIS:N	1:I:238:LEU:O	2.37	0.45	
1:M:287:VAL:HG12	1:P:213:PRO:HD2	1.99	0.45	
1:I:12:ARG:HB2	2:I:401:NAD:O1N	2.17	0.45	
1:J:138:VAL:HG23	1:J:225:VAL:HG11	1.98	0.45	
1:A:39:ASP:OD1	1:A:40:ILE:N	2.48	0.45	
1:D:170:LEU:HD13	1:D:252:VAL:HG11	1.99	0.45	
1:F:202:ARG:NH1	1:G:286:ILE:O	2.48	0.45	
1:I:25:GLN:NE2	1:I:32:VAL:O	2.49	0.45	
1:J:211:ILE:HG22	1:J:240:VAL:HA	1.99	0.45	
1:L:91:PRO:HB2	1:L:94:ASP:HB2	1.99	0.45	
1:M:12:ARG:HG3	1:O:194:GLN:HG2	1.99	0.45	
1:N:163:LEU:HD22	1:N:181:MET:SD	2.57	0.45	
1:H:39:ASP:OD1	1:H:40:ILE:N	2.50	0.45	
1:A:100:VAL:HG11	1:A:116:HIS:ND1	2.32	0.45	
1:J:236:TYR:HE1	1:K:313:LYS:HD3	1.81	0.45	
1:J:313:LYS:HE3	1:K:180:LEU:HB3	1.98	0.45	
1:L:25:GLN:NE2	1:L:32:VAL:O	2.49	0.45	
1:N:271:ALA:HB2	1:N:279:LEU:HD22	1.99	0.45	
1:O:213:PRO:HB3	1:O:238:LEU:HD21	1.98	0.45	
1:K:260:VAL:HG23	1:K:307:VAL:HG12	1.99	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:39:ASP:HA	2:L:401:NAD:H8A	1.98	0.45
1:B:144:ASP:OD1	1:B:144:ASP:N	2.50	0.44
1:F:54:SER:N	1:H:205:ARG:HH12	2.14	0.44
1:F:280:LYS:HE3	1:F:282:TYR:HE2	1.82	0.44
1:B:280:LYS:HB2	1:B:296:HIS:ND1	2.33	0.44
1:D:100:VAL:HG11	1:D:116:HIS:ND1	2.32	0.44
1:F:322:TRP:O	1:F:326:ASN:ND2	2.38	0.44
1:N:17:PHE:HA	1:N:325:SER:HB3	1.98	0.44
1:G:211:ILE:HG23	1:G:240:VAL:HG12	2.00	0.44
1:A:170:LEU:HD13	1:A:252:VAL:HG11	1.99	0.44
1:D:190:ASP:OD2	1:D:203:ARG:NH1	2.51	0.44
1:F:170:LEU:HD13	1:F:252:VAL:HG11	2.00	0.44
1:M:69:ASP:HA	1:M:79:LYS:H	1.82	0.44
1:C:170:LEU:HD13	1:C:252:VAL:HG11	2.00	0.44
1:F:141:VAL:HG21	1:F:164:ALA:HB1	1.99	0.44
1:H:190:ASP:OD1	1:H:203:ARG:NH1	2.50	0.44
1:F:248:THR:HG23	1:F:318:TYR:CE1	2.53	0.44
1:I:143:ASP:N	1:I:143:ASP:OD1	2.51	0.44
1:I:322:TRP:O	1:I:326:ASN:ND2	2.39	0.44
1:N:240:VAL:O	1:N:242:ILE:N	2.50	0.44
1:O:289:SER:HB3	1:P:54:SER:HA	1.99	0.44
1:A:213:PRO:HG3	1:D:317:TRP:HZ2	1.83	0.44
1:E:320:ASN:O	2:E:401:NAD:H4N	2.18	0.44
1:G:73:VAL:C	1:G:75:ARG:H	2.21	0.44
1:D:39:ASP:HA	2:D:401:NAD:C8A	2.48	0.44
1:D:110:ALA:HA	1:D:113:ALA:HB3	1.99	0.44
1:E:291:ILE:HG23	1:E:299:ILE:HD12	2.00	0.44
1:M:313:LYS:HE2	1:P:180:LEU:HB3	2.00	0.44
1:O:4:ARG:HD3	1:O:96:GLY:O	2.18	0.44
1:O:267:PHE:HD1	1:O:279:LEU:HD21	1.81	0.44
1:A:143:ASP:OD1	1:A:143:ASP:N	2.51	0.43
1:F:59:LEU:HD12	1:F:60:PRO:HD2	1.99	0.43
1:M:166:LEU:HD21	1:M:316:SER:HB2	1.99	0.43
1:B:100:VAL:HG11	1:B:116:HIS:ND1	2.33	0.43
1:C:4:ARG:HD3	1:C:96:GLY:O	2.18	0.43
1:F:143:ASP:OD1	1:F:143:ASP:N	2.51	0.43
1:I:213:PRO:HG3	1:L:317:TRP:HZ2	1.82	0.43
1:K:54:SER:HA	1:L:289:SER:HB3	2.00	0.43
1:N:53:ASP:C	1:P:205:ARG:HH22	2.22	0.43
1:B:170:LEU:HD13	1:B:252:VAL:HG11	2.00	0.43
1:D:246:SER:HB2	1:D:318:TYR:CZ	2.53	0.43



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:291:ILE:HD12	1:E:299:ILE:HD12	2.00	0.43
1:F:211:ILE:HG22	1:F:240:VAL:HG12	2.00	0.43
1:H:10:PHE:HD2	1:H:46:LEU:HD22	1.83	0.43
1:K:100:VAL:HG11	1:K:116:HIS:ND1	2.33	0.43
1:L:143:ASP:N	1:L:143:ASP:OD1	2.52	0.43
1:G:322:TRP:O	1:G:326:ASN:ND2	2.44	0.43
1:I:58:ARG:NE	1:J:290:ASP:O	2.52	0.43
1:N:242:ILE:HD11	1:O:211:ILE:HG23	2.01	0.43
1:E:170:LEU:HD11	1:E:314:VAL:HG21	1.99	0.43
1:F:211:ILE:HG22	1:F:240:VAL:HA	1.99	0.43
1:G:143:ASP:N	1:G:143:ASP:OD1	2.51	0.43
1:H:240:VAL:O	1:H:242:ILE:N	2.51	0.43
1:K:143:ASP:OD1	1:K:143:ASP:N	2.51	0.43
1:B:209:LEU:HD11	1:D:243:PRO:HB3	2.00	0.43
1:C:288:SER:HB3	1:C:317:TRP:CZ3	2.53	0.43
1:E:287:VAL:HG12	1:H:213:PRO:HD2	2.01	0.43
1:I:183:THR:HG1	1:I:318:TYR:HH	1.61	0.43
1:K:300:PHE:CE1	1:K:314:VAL:HG13	2.53	0.43
1:L:155:ASN:ND2	1:L:155:ASN:O	2.51	0.43
1:M:139:LEU:HA	1:M:143:ASP:HB3	2.00	0.43
1:P:143:ASP:OD1	1:P:143:ASP:N	2.51	0.43
1:F:310:ASP:H	1:G:178:LYS:HE3	1.83	0.43
1:I:166:LEU:HD21	1:I:316:SER:HB2	2.01	0.43
1:J:143:ASP:OD1	1:J:143:ASP:N	2.52	0.43
1:O:248:THR:HG23	1:O:318:TYR:CE1	2.54	0.43
1:A:141:VAL:HG21	1:A:164:ALA:HB1	2.00	0.43
1:C:19:ARG:NH2	1:C:50:LEU:O	2.52	0.43
1:F:280:LYS:HB3	1:F:299:ILE:HD13	2.01	0.43
1:I:291:ILE:HG21	1:I:317:TRP:HB3	2.01	0.43
1:K:170:LEU:HD11	1:K:314:VAL:HG21	2.01	0.43
1:N:107:PHE:HD1	1:N:112:LYS:HD3	1.83	0.43
1:E:178:LYS:HD2	1:H:309:ASP:HB3	2.01	0.42
1:N:73:VAL:C	1:N:75:ARG:H	2.23	0.42
1:P:38:ASN:HA	1:P:81:LEU:HA	2.01	0.42
1:C:202:ARG:HD2	1:C:213:PRO:HG2	1.99	0.42
1:I:12:ARG:HG3	1:K:194:GLN:HG2	2.00	0.42
1:L:248:THR:HG23	1:L:318:TYR:CE1	2.54	0.42
1:D:297:SER:HB2	1:D:327:ARG:HH11	1.85	0.42
1:E:92:TRP:HE1	1:E:116:HIS:HD1	1.65	0.42
1:K:294:ASP:OD2	1:L:58:ARG:NH1	2.52	0.42
1:M:143:ASP:OD1	1:M:143:ASP:N	2.52	0.42



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:N:320:ASN:HD22	2:N:401:NAD:H72N	1.68	0.42	
1:B:180:LEU:HB3	1:C:313:LYS:HE2	2.00	0.42	
1:F:144:ASP:OD1	1:F:144:ASP:N	2.52	0.42	
1:L:188:THR:OG1	1:L:239:ARG:NH1	2.52	0.42	
1:M:92:TRP:HE1	1:M:116:HIS:HD1	1.66	0.42	
1:0:143:ASP:OD1	1:O:143:ASP:N	2.52	0.42	
1:B:291:ILE:HD12	1:B:299:ILE:HD12	2.01	0.42	
1:C:143:ASP:OD1	1:C:143:ASP:N	2.52	0.42	
1:G:92:TRP:HD1	1:G:119:ALA:HB3	1.84	0.42	
1:G:190:ASP:OD1	1:G:203:ARG:NH1	2.52	0.42	
1:H:12:ARG:HH11	1:H:15:ARG:HH21	1.65	0.42	
1:J:38:ASN:ND2	2:J:401:NAD:H2A	2.34	0.42	
1:A:58:ARG:NH1	1:B:294:ASP:OD2	2.53	0.42	
1:C:110:ALA:HA	1:C:113:ALA:HB3	2.02	0.42	
1:H:143:ASP:OD1	1:H:143:ASP:N	2.53	0.42	
1:I:313:LYS:HE2	1:L:180:LEU:HB3	2.01	0.42	
1:K:10:PHE:HD2	1:K:46:LEU:HD22	1.85	0.42	
1:O:163:LEU:HD22	1:O:181:MET:SD	2.60	0.42	
1:P:12:ARG:HH11	1:P:15:ARG:HH21	1.68	0.42	
1:H:163:LEU:HD22	1:H:181:MET:SD	2.60	0.42	
1:L:39:ASP:HA	2:L:401:NAD:C8A	2.49	0.42	
1:M:211:ILE:HG23	1:P:242:ILE:HD12	2.02	0.42	
1:N:313:LYS:HE2	1:O:180:LEU:HB3	2.02	0.42	
1:B:143:ASP:OD1	1:B:143:ASP:N	2.52	0.42	
1:E:293:THR:N	1:E:319:ASP:OD2	2.50	0.42	
1:H:248:THR:HG23	1:H:318:TYR:CE1	2.55	0.42	
1:I:248:THR:HG23	1:I:318:TYR:CE1	2.54	0.42	
1:P:291:ILE:HD12	1:P:299:ILE:HD12	2.02	0.42	
1:A:190:ASP:OD2	1:A:203:ARG:NH1	2.53	0.42	
1:B:110:ALA:HA	1:B:113:ALA:HB3	2.01	0.42	
1:B:188:THR:OG1	1:B:239:ARG:NH1	2.53	0.42	
1:I:17:PHE:HA	1:I:325:SER:HB3	2.01	0.42	
1:K:85:GLU:OE1	1:K:85:GLU:N	2.53	0.42	
1:K:202:ARG:HD2	1:K:213:PRO:HG2	2.02	0.42	
1:N:180:LEU:HB3	1:O:313:LYS:HE2	2.01	0.42	
2:E:401:NAD:H2N	2:E:401:NAD:H2D	1.73	0.41	
1:K:9:GLY:O	1:K:103:SER:OG	2.31	0.41	
1:O:166:LEU:HA	1:O:267:PHE:HE1	1.85	0.41	
1:O:188:THR:OG1	1:O:239:ARG:NH1	2.43	0.41	
1:B:55:ILE:HD13	1:B:244:THR:HG23	2.02	0.41	
1:C:260:VAL:HG23	1:C:307:VAL:HG12	2.03	0.41	



	t i c	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:143:ASP:OD1	1:E:143:ASP:N	2.50	0.41	
1:E:313:LYS:HD3	1:H:236:TYR:HE1	1.86	0.41	
1:I:100:VAL:HG11	1:I:116:HIS:ND1	2.35	0.41	
1:0:213:PRO:CA	1:O:238:LEU:HD23	2.50	0.41	
1:B:59:LEU:HD12	1:B:60:PRO:HD2	2.02	0.41	
1:C:100:VAL:HG11	1:C:116:HIS:ND1	2.36	0.41	
1:E:73:VAL:C	1:E:75:ARG:H	2.23	0.41	
1:J:280:LYS:HB2	1:J:296:HIS:CD2	2.55	0.41	
1:0:68:ASP:OD1	1:O:68:ASP:N	2.52	0.41	
1:C:112:LYS:HE2	1:E:269:ALA:HB2	2.02	0.41	
1:C:289:SER:HB3	1:D:54:SER:HA	2.02	0.41	
1:D:139:LEU:HD21	1:D:331:LEU:HD13	2.03	0.41	
1:E:186:ALA:HB2	1:E:245:GLY:O	2.19	0.41	
1:H:188:THR:OG1	1:H:239:ARG:NH1	2.51	0.41	
1:I:92:TRP:HD1	1:I:119:ALA:HB3	1.84	0.41	
1:M:211:ILE:HG23	1:P:242:ILE:CD1	2.50	0.41	
1:A:307:VAL:HG23	1:A:312:ALA:HB2	2.01	0.41	
1:C:38:ASN:ND2	2:C:401:NAD:H2A	2.36	0.41	
1:H:257:ARG:NH2	1:N:231:GLY:HA3	2.35	0.41	
1:J:240:VAL:O	1:J:242:ILE:N	2.54	0.41	
1:M:289:SER:HB3	1:P:210:ASN:HB3	2.03	0.41	
1:N:143:ASP:OD1	1:N:143:ASP:N	2.51	0.41	
1:O:59:LEU:HD12	1:O:60:PRO:HD2	2.02	0.41	
1:A:181:MET:HG3	1:A:235:GLY:HA3	2.02	0.41	
1:D:186:ALA:HA	1:D:242:ILE:HG22	2.02	0.41	
1:H:155:ASN:HB3	1:H:324:TYR:OH	2.20	0.41	
1:J:280:LYS:HB3	1:J:299:ILE:HG23	2.03	0.41	
1:C:322:TRP:O	1:C:326:ASN:ND2	2.46	0.41	
1:E:17:PHE:HA	1:E:325:SER:HB3	2.02	0.41	
1:I:9:GLY:HA2	2:I:401:NAD:H8A	2.02	0.41	
1:M:3:VAL:HG21	1:M:336:GLY:HA3	2.03	0.41	
1:P:240:VAL:O	1:P:242:ILE:N	2.52	0.41	
1:D:39:ASP:HA	2:D:401:NAD:H8A	2.03	0.41	
1:D:300:PHE:HE1	1:D:314:VAL:HG13	1.86	0.41	
1:F:15:ARG:NH2	1:H:195:ASP:O	2.38	0.41	
1:F:313:LYS:HE2	1:G:180:LEU:HB3	2.02	0.41	
1:I:211:ILE:HG22	1:I:240:VAL:HA	2.03	0.41	
2:I:401:NAD:N3A	2:I:401:NAD:H2B	2.36	0.41	
1:L:68:ASP:N	1:L:68:ASP:OD1	2.53	0.41	
1:M:87:PRO:HD3	1:M:107:PHE:CZ	2.55	0.41	
1:M:100:VAL:HG11	1:M:116:HIS:ND1	2.36	0.41	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:N:4:ARG:HD3	1:N:96:GLY:O	2.21	0.41
1:O:126:ILE:HG22	1:O:128:ALA:H	1.84	0.41
1:A:271:ALA:HB2	1:A:279:LEU:HD22	2.03	0.41
1:B:190:ASP:OD1	1:B:203:ARG:NH1	2.54	0.41
1:M:12:ARG:HH21	1:M:55:ILE:HD12	1.85	0.41
1:M:54:SER:OG	1:O:205:ARG:NH1	2.53	0.41
1:M:186:ALA:HB1	1:M:242:ILE:O	2.21	0.41
1:N:100:VAL:HG11	1:N:116:HIS:ND1	2.36	0.41
1:P:246:SER:HB2	1:P:318:TYR:CZ	2.56	0.41
1:A:104:THR:HA	2:A:401:NAD:H52A	2.02	0.40
1:A:248:THR:HG23	1:A:318:TYR:CE1	2.56	0.40
1:D:39:ASP:OD1	2:D:401:NAD:H1B	2.22	0.40
1:D:59:LEU:HD12	1:D:60:PRO:HD2	2.02	0.40
1:D:248:THR:HG23	1:D:318:TYR:CE1	2.56	0.40
1:F:307:VAL:HG23	1:F:312:ALA:HB2	2.02	0.40
1:B:10:PHE:CE2	1:B:15:ARG:HG2	2.57	0.40
1:M:92:TRP:HD1	1:M:119:ALA:HB3	1.85	0.40
1:B:249:ASP:OD1	1:B:313:LYS:NZ	2.37	0.40
1:D:143:ASP:OD1	1:D:143:ASP:N	2.52	0.40
1:F:92:TRP:HD1	1:F:119:ALA:HB3	1.85	0.40
1:I:213:PRO:HD2	1:L:287:VAL:HG12	2.03	0.40
1:M:17:PHE:HA	1:M:325:SER:HB3	2.04	0.40
1:B:238:LEU:HD13	1:C:184:ILE:HD12	2.02	0.40
1:M:240:VAL:HG21	1:P:211:ILE:HD11	2.02	0.40
1:B:280:LYS:HB2	1:B:296:HIS:CE1	2.56	0.40
1:E:202:ARG:NH1	1:H:286:ILE:O	2.53	0.40
1:I:222:ILE:HG21	1:I:233:LEU:HD12	2.04	0.40
1:J:59:LEU:HD12	1:J:60:PRO:HD2	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	Perce	entiles
1	А	337/357~(94%)	313~(93%)	22~(6%)	2(1%)	25	57
1	В	336/357~(94%)	309~(92%)	26 (8%)	1 (0%)	41	71
1	С	337/357~(94%)	310 (92%)	26 (8%)	1 (0%)	41	71
1	D	336/357~(94%)	311 (93%)	23~(7%)	2(1%)	25	57
1	Ε	337/357~(94%)	313 (93%)	22~(6%)	2(1%)	25	57
1	F	336/357~(94%)	307~(91%)	28 (8%)	1 (0%)	41	71
1	G	337/357~(94%)	310 (92%)	26 (8%)	1 (0%)	41	71
1	Н	336/357~(94%)	309 (92%)	26 (8%)	1 (0%)	41	71
1	Ι	337/357~(94%)	311 (92%)	24 (7%)	2(1%)	25	57
1	J	336/357~(94%)	308 (92%)	27 (8%)	1 (0%)	41	71
1	Κ	337/357~(94%)	315~(94%)	19 (6%)	3~(1%)	17	48
1	L	336/357~(94%)	306 (91%)	29 (9%)	1 (0%)	41	71
1	М	337/357~(94%)	310 (92%)	26 (8%)	1 (0%)	41	71
1	Ν	336/357~(94%)	311 (93%)	22 (6%)	3 (1%)	17	48
1	Ο	337/357~(94%)	313 (93%)	22~(6%)	2(1%)	25	57
1	Р	336/357~(94%)	311 (93%)	23 (7%)	2 (1%)	25	57
All	All	5384/5712~(94%)	4967 (92%)	391 (7%)	26 (0%)	29	61

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	72	VAL
1	С	72	VAL
1	D	72	VAL
1	Е	72	VAL
1	F	72	VAL
1	G	72	VAL
1	Н	72	VAL
1	Ι	72	VAL
1	J	72	VAL
1	Κ	72	VAL
1	L	72	VAL
1	М	72	VAL
1	Ν	72	VAL
1	Р	72	VAL
1	Р	244	THR
1	0	73	VAL



Mol	Chain	Res	Type
1	В	72	VAL
1	Κ	243	PRO
1	0	80	ALA
1	Ι	40	ILE
1	Ν	243	PRO
1	А	40	ILE
1	D	83	VAL
1	N	241	PRO
1	Е	74	GLY
1	К	40	ILE

#### 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	Perce	ntiles
1	А	220/284~(78%)	220 (100%)	0	100	100
1	В	223/284~(78%)	222 (100%)	1 (0%)	91	95
1	С	215/284~(76%)	214 (100%)	1 (0%)	88	93
1	D	217/284~(76%)	216 (100%)	1 (0%)	88	93
1	Ε	222/284~(78%)	222 (100%)	0	100	100
1	F	225/284~(79%)	224 (100%)	1 (0%)	91	95
1	G	214/284~(75%)	213 (100%)	1 (0%)	88	93
1	Н	220/284~(78%)	220 (100%)	0	100	100
1	Ι	221/284~(78%)	221 (100%)	0	100	100
1	J	225/284~(79%)	225 (100%)	0	100	100
1	К	213/284~(75%)	212 (100%)	1 (0%)	88	93
1	L	216/284~(76%)	215 (100%)	1 (0%)	88	93
1	М	220/284~(78%)	219 (100%)	1 (0%)	88	93
1	N	$22\overline{3}/284~(78\%)$	223 (100%)	0	100	100
1	Ο	211/284 (74%)	210 (100%)	1 (0%)	88	93
1	Р	217/284~(76%)	216 (100%)	1 (0%)	88	93



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
All	All	3502/4544~(77%)	3492 (100%)	10 (0%)	92	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	58	ARG
1	С	310	ASP
1	D	282	TYR
1	F	282	TYR
1	G	282	TYR
1	Κ	154	SER
1	L	282	TYR
1	М	189	GLN
1	0	282	TYR
1	Р	282	TYR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

18 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


Mol	Tuno	Chain	Dog	Link	Bo	ond leng	nd lengths		Bond angles		
	туре	Unain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	EDO	D	402	-	3,3,3	0.46	0	$2,\!2,\!2$	0.34	0	
3	EDO	А	402	-	3,3,3	0.46	0	2,2,2	0.34	0	
2	NAD	L	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.87	2 (4%)	
2	NAD	В	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.87	3 (6%)	
2	NAD	А	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.92	3 (6%)	
2	NAD	С	401	-	42,48,48	0.69	1 (2%)	50,73,73	0.84	2 (4%)	
2	NAD	Е	401	-	42,48,48	0.72	1 (2%)	50,73,73	0.90	3 (6%)	
2	NAD	D	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.85	2 (4%)	
2	NAD	Ι	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.90	2 (4%)	
2	NAD	М	401	-	42,48,48	0.68	1 (2%)	50,73,73	0.98	4 (8%)	
2	NAD	G	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.80	2 (4%)	
2	NAD	N	401	-	42,48,48	0.69	1 (2%)	50,73,73	0.85	2 (4%)	
2	NAD	Р	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.87	2 (4%)	
2	NAD	Н	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.87	2 (4%)	
2	NAD	K	401	-	42,48,48	0.70	1 (2%)	50,73,73	0.83	2 (4%)	
2	NAD	J	401	-	42,48,48	0.69	1 (2%)	50,73,73	0.85	2 (4%)	
2	NAD	Ο	401	-	42,48,48	0.68	1 (2%)	50,73,73	0.89	2 (4%)	
2	NAD	F	401	-	42,48,48	0.71	1 (2%)	50,73,73	0.83	3 (6%)	

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).

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	402	-	-	1/1/1/1	-
3	EDO	А	402	-	-	0/1/1/1	-
2	NAD	L	401	-	-	5/26/62/62	0/5/5/5
2	NAD	В	401	-	-	7/26/62/62	0/5/5/5
2	NAD	А	401	-	-	9/26/62/62	0/5/5/5
2	NAD	С	401	-	-	5/26/62/62	0/5/5/5
2	NAD	Е	401	-	-	13/26/62/62	0/5/5/5
2	NAD	D	401	-	-	5/26/62/62	0/5/5/5
2	NAD	Ι	401	-	-	7/26/62/62	0/5/5/5



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	М	401	-	-	12/26/62/62	0/5/5/5
2	NAD	G	401	-	-	6/26/62/62	0/5/5/5
2	NAD	Ν	401	-	-	5/26/62/62	0/5/5/5
2	NAD	Р	401	-	-	9/26/62/62	0/5/5/5
2	NAD	Н	401	-	-	5/26/62/62	0/5/5/5
2	NAD	K	401	-	-	5/26/62/62	0/5/5/5
2	NAD	J	401	-	-	5/26/62/62	0/5/5/5
2	NAD	Ο	401	-	-	5/26/62/62	0/5/5/5
2	NAD	F	401	-	-	13/26/62/62	0/5/5/5

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All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	А	401	NAD	C2N-N1N	2.59	1.38	1.35
2	Е	401	NAD	C2N-N1N	2.59	1.38	1.35
2	L	401	NAD	C2N-N1N	2.59	1.38	1.35
2	С	401	NAD	C2N-N1N	2.58	1.38	1.35
2	Н	401	NAD	C2N-N1N	2.57	1.38	1.35
2	Κ	401	NAD	C2N-N1N	2.57	1.38	1.35
2	Р	401	NAD	C2N-N1N	2.57	1.38	1.35
2	F	401	NAD	C2N-N1N	2.56	1.38	1.35
2	Ι	401	NAD	C2N-N1N	2.56	1.38	1.35
2	G	401	NAD	C2N-N1N	2.56	1.38	1.35
2	D	401	NAD	C2N-N1N	2.55	1.38	1.35
2	J	401	NAD	C2N-N1N	2.55	1.38	1.35
2	Ν	401	NAD	C2N-N1N	2.55	1.38	1.35
2	В	401	NAD	C2N-N1N	2.55	1.38	1.35
2	М	401	NAD	C2N-N1N	2.51	1.38	1.35
2	0	401	NAD	C2N-N1N	2.51	1.38	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	М	401	NAD	O4B-C1B-C2B	-3.26	102.16	106.93
2	В	401	NAD	O4B-C1B-C2B	-3.04	102.48	106.93
2	0	401	NAD	O4B-C1B-C2B	-3.01	102.53	106.93
2	Е	401	NAD	O4B-C1B-C2B	-2.91	102.68	106.93
2	Н	401	NAD	O4B-C1B-C2B	-2.90	102.69	106.93
2	L	401	NAD	O4B-C1B-C2B	-2.86	102.75	106.93
2	Р	401	NAD	O4B-C1B-C2B	-2.85	102.77	106.93

B



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	J	401	NAD	O4B-C1B-C2B	-2.83	102.79	106.93
2	K	401	NAD	O4B-C1B-C2B	-2.82	102.80	106.93
2	С	401	NAD	O4B-C1B-C2B	-2.82	102.81	106.93
2	N	401	NAD	O4B-C1B-C2B	-2.81	102.81	106.93
2	М	401	NAD	O4D-C1D-C2D	-2.79	102.85	106.93
2	D	401	NAD	O4B-C1B-C2B	-2.78	102.87	106.93
2	А	401	NAD	O4B-C1B-C2B	-2.70	102.98	106.93
2	Ι	401	NAD	O4B-C1B-C2B	-2.69	103.00	106.93
2	F	401	NAD	O4B-C1B-C2B	-2.50	103.27	106.93
2	В	401	NAD	C5A-C6A-N6A	2.36	123.94	120.35
2	0	401	NAD	C5A-C6A-N6A	2.34	123.91	120.35
2	N	401	NAD	C5A-C6A-N6A	2.30	123.85	120.35
2	G	401	NAD	C5A-C6A-N6A	2.27	123.81	120.35
2	F	401	NAD	C5A-C6A-N6A	2.27	123.80	120.35
2	J	401	NAD	C5A-C6A-N6A	2.27	123.80	120.35
2	K	401	NAD	C5A-C6A-N6A	2.26	123.79	120.35
2	С	401	NAD	C5A-C6A-N6A	2.25	123.77	120.35
2	Н	401	NAD	C5A-C6A-N6A	2.21	123.70	120.35
2	D	401	NAD	C5A-C6A-N6A	2.20	123.70	120.35
2	А	401	NAD	C5A-C6A-N6A	2.20	123.70	120.35
2	L	401	NAD	C5A-C6A-N6A	2.20	123.69	120.35
2	Ι	401	NAD	C5A-C6A-N6A	2.20	123.69	120.35
2	Р	401	NAD	C5A-C6A-N6A	2.20	123.69	120.35
2	М	401	NAD	C5A-C6A-N6A	2.18	123.66	120.35
2	Е	401	NAD	C5A-C6A-N6A	2.15	123.62	120.35
2	Е	401	NAD	C6N-N1N-C2N	-2.11	120.06	121.97
2	G	401	NAD	O4B-C1B-C2B	-2.10	103.86	106.93
2	М	401	NAD	C1B-N9A-C4A	2.05	130.25	126.64
2	В	401	NAD	C6N-N1N-C2N	-2.03	120.12	121.97
2	А	401	NAD	C6N-N1N-C2N	-2.02	120.14	121.97
2	F	401	NAD	C6N-N1N-C2N	-2.01	120.15	121.97

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There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	401	NAD	O4B-C4B-C5B-O5B
2	А	401	NAD	C5D-O5D-PN-O2N
2	В	401	NAD	O4D-C1D-N1N-C2N
2	В	401	NAD	O4D-C1D-N1N-C6N
2	В	401	NAD	C2D-C1D-N1N-C2N
2	В	401	NAD	C2D-C1D-N1N-C6N



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Mol	Chain	Res	Type	Atoms
2	С	401	NAD	O4D-C1D-N1N-C2N
2	С	401	NAD	O4D-C1D-N1N-C6N
2	С	401	NAD	C2D-C1D-N1N-C2N
2	С	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	Е	401	NAD	C5B-O5B-PA-O1A
2	Е	401	NAD	C5B-O5B-PA-O2A
2	Е	401	NAD	O4B-C4B-C5B-O5B
2	Е	401	NAD	O4D-C1D-N1N-C2N
2	Е	401	NAD	O4D-C1D-N1N-C6N
2	Е	401	NAD	C2D-C1D-N1N-C2N
2	Е	401	NAD	C2D-C1D-N1N-C6N
2	F	401	NAD	PN-O3-PA-O5B
2	F	401	NAD	C5D-O5D-PN-O1N
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	C2D-C1D-N1N-C2N
2	G	401	NAD	C2D-C1D-N1N-C6N
2	Н	401	NAD	O4D-C1D-N1N-C2N
2	Н	401	NAD	O4D-C1D-N1N-C6N
2	Н	401	NAD	C2D-C1D-N1N-C2N
2	Н	401	NAD	C2D-C1D-N1N-C6N
2	Ι	401	NAD	PA-O3-PN-O5D
2	Ι	401	NAD	C5D-O5D-PN-O2N
2	J	401	NAD	O4D-C1D-N1N-C2N
2	J	401	NAD	O4D-C1D-N1N-C6N
2	J	401	NAD	C2D-C1D-N1N-C2N
2	J	401	NAD	C2D-C1D-N1N-C6N
2	K	401	NAD	O4D-C1D-N1N-C2N
2	K	401	NAD	O4D-C1D-N1N-C6N
2	K	401	NAD	C2D-C1D-N1N-C2N
2	K	401	NAD	C2D-C1D-N1N-C6N
2	L	401	NAD	O4D-C1D-N1N-C2N
2	L	401	NAD	O4D-C1D-N1N-C6N
2	Γ	401	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	L	401	NAD	C2D-C1D-N1N-C6N
2	М	401	NAD	C5B-O5B-PA-O3
2	М	401	NAD	O4B-C4B-C5B-O5B
2	М	401	NAD	C5D-O5D-PN-O2N
2	М	401	NAD	O4D-C4D-C5D-O5D
2	М	401	NAD	C3D-C4D-C5D-O5D
2	N	401	NAD	O4D-C1D-N1N-C2N
2	N	401	NAD	O4D-C1D-N1N-C6N
2	Ν	401	NAD	C2D-C1D-N1N-C2N
2	Ν	401	NAD	C2D-C1D-N1N-C6N
2	0	401	NAD	O4D-C1D-N1N-C2N
2	0	401	NAD	O4D-C1D-N1N-C6N
2	0	401	NAD	C2D-C1D-N1N-C6N
2	Р	401	NAD	C5B-O5B-PA-O1A
2	Р	401	NAD	O4D-C1D-N1N-C2N
2	Р	401	NAD	O4D-C1D-N1N-C6N
2	Р	401	NAD	C2D-C1D-N1N-C2N
2	Р	401	NAD	C2D-C1D-N1N-C6N
2	А	401	NAD	C3D-C4D-C5D-O5D
2	Е	401	NAD	O4D-C4D-C5D-O5D
2	F	401	NAD	O4D-C4D-C5D-O5D
2	Ι	401	NAD	O4B-C4B-C5B-O5B
2	А	401	NAD	C3B-C4B-C5B-O5B
2	А	401	NAD	O4D-C4D-C5D-O5D
2	E	401	NAD	C3B-C4B-C5B-O5B
2	F	401	NAD	C3D-C4D-C5D-O5D
2	I	401	NAD	C3B-C4B-C5B-O5B
2	М	401	NAD	C3B-C4B-C5B-O5B
2	E	401	NAD	C3D-C4D-C5D-O5D
2	A	401	NAD	PA-O3-PN-O5D
2	E	401	NAD	PN-O3-PA-O5B
2	М	401	NAD	PN-O3-PA-O5B
2	I	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	C5D-O5D-PN-O3
2	I	401	NAD	C5D-O5D-PN-O3
2	M	401	NAD	C5D-O5D-PN-O3
2	P	401	NAD	C5B-O5B-PA-O3
2	F	401	NAD	PA-O3-PN-O2N
2	A	401	NAD	C4B-C5B-O5B-PA
2	M	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	C5D-O5D-PN-O1N
2	I	401	NAD	C5D-O5D-PN-O1N

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	v	1	1 0	
Mol	Chain	Res	Type	Atoms
2	М	401	NAD	C5B-O5B-PA-O2A
2	М	401	NAD	C5D-O5D-PN-O1N
2	Р	401	NAD	C5B-O5B-PA-O2A
3	D	402	EDO	O1-C1-C2-O2
2	Е	401	NAD	C4B-C5B-O5B-PA
2	В	401	NAD	PN-O3-PA-O1A
2	М	401	NAD	C4D-C5D-O5D-PN
2	F	401	NAD	O4B-C4B-C5B-O5B
2	Р	401	NAD	C4B-C5B-O5B-PA
2	Р	401	NAD	O4B-C4B-C5B-O5B
2	Е	401	NAD	C5B-O5B-PA-O3
2	F	401	NAD	C5B-O5B-PA-O3
2	F	401	NAD	C5D-O5D-PN-O3
2	0	401	NAD	C2D-C1D-N1N-C2N
2	В	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	O4B-C4B-C5B-O5B
2	Н	401	NAD	O4B-C4B-C5B-O5B
2	L	401	NAD	O4B-C4B-C5B-O5B
2	N	401	NAD	O4B-C4B-C5B-O5B
2	0	401	NAD	O4B-C4B-C5B-O5B
2	В	401	NAD	PN-O3-PA-O2A
2	F	401	NAD	PA-O3-PN-O1N
2	G	401	NAD	PN-O3-PA-O2A
2	С	401	NAD	O4B-C4B-C5B-O5B
2	G	401	NAD	O4B-C4B-C5B-O5B
2	J	401	NAD	O4B-C4B-C5B-O5B
2	K	401	NAD	O4B-C4B-C5B-O5B

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There are no ring outliers.

14 monomers are	involved	in $32$	$\operatorname{short}$	contacts:
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	401	NAD	2	0
2	В	401	NAD	2	0
2	А	401	NAD	4	0
2	С	401	NAD	1	0
2	Е	401	NAD	3	0
2	D	401	NAD	3	0
2	Ι	401	NAD	5	0
2	М	401	NAD	2	0
2	Ν	401	NAD	1	0
2	Р	401	NAD	2	0



	0	-	1 0		
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	401	NAD	2	0
2	J	401	NAD	2	0
2	0	401	NAD	2	0
2	F	401	NAD	1	0

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The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





























































# 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 (i)

# 6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	339/357~(94%)	0.01	3 (0%) 84 84	30, 47, 61, 77	0
1	В	338/357~(94%)	0.11	10 (2%) 50 49	33,  46,  63,  71	0
1	С	339/357~(94%)	0.19	14 (4%) 37 35	29, 47, 68, 85	0
1	D	338/357~(94%)	0.18	6 (1%) 68 67	33, 53, 67, 78	0
1	Е	339/357~(94%)	0.01	3 (0%) 84 84	33, 43, 58, 69	0
1	F	338/357~(94%)	0.16	7 (2%) 63 62	30, 47, 60, 77	0
1	G	339/357~(94%)	0.17	11 (3%) 47 46	29, 47, 63, 75	0
1	Н	338/357~(94%)	0.20	7 (2%) 63 62	33, 48, 63, 73	0
1	Ι	339/357~(94%)	0.12	7 (2%) 63 62	31, 47, 63, 75	0
1	J	338/357~(94%)	0.40	18 (5%) 26 24	39,56,71,84	0
1	Κ	339/357~(94%)	0.27	11 (3%) 47 46	39,56,70,81	0
1	L	338/357~(94%)	0.20	6 (1%) 68 67	35, 47, 62, 73	0
1	М	339/357~(94%)	0.23	7 (2%) 63 62	35, 57, 69, 85	0
1	Ν	338/357~(94%)	0.23	9 (2%) 54 52	36, 56, 72, 81	0
1	Ο	339/357~(94%)	0.49	21 (6%) 20 20	38, 66, 84, 104	0
1	Р	$33\overline{8/357}~(94\%)$	0.18	3 (0%) 84 84	34, 53, 67, 80	0
All	All	5416/5712 (94%)	0.20	143 (2%) 56 53	29, 50, 70, 104	0

#### All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Р	80	ALA	5.3
1	0	179	GLY	4.8
1	С	34	VAL	4.8
1	0	99	VAL	4.4
1	В	82	ALA	3.9



Mol	Chain	Res	Type	RSRZ
1	С	98	ASP	3.9
1	D	82	ALA	3.8
1	0	219	ALA	3.8
1	А	30	ALA	3.6
1	В	153	ILE	3.5
1	Ν	82	ALA	3.5
1	J	165	PRO	3.5
1	Ι	97	VAL	3.5
1	Н	82	ALA	3.4
1	С	92	TRP	3.4
1	Ν	339	LEU	3.4
1	D	118	ASP	3.4
1	С	151	ASN	3.4
1	0	255	SER	3.3
1	N	311	GLN	3.3
1	Н	108	THR	3.3
1	J	311	GLN	3.3
1	В	124	VAL	3.2
1	С	65	LEU	3.2
1	Ν	179	GLY	3.1
1	М	82	ALA	3.1
1	0	235	GLY	3.1
1	G	338	SER	3.1
1	0	153	ILE	3.0
1	М	92	TRP	3.0
1	Р	2	THR	3.0
1	K	127	SER	3.0
1	С	66	GLU	3.0
1	D	258	ALA	2.9
1	0	125	ILE	2.9
1	0	124	VAL	2.9
1	Н	252	VAL	2.9
1	G	99	VAL	2.8
1	F	127	SER	2.8
1	L	82	ALA	2.8
1	0	5	VAL	2.8
1	J	332	VAL	2.7
1	F	137	ILE	2.7
1	С	35	VAL	2.7
1	0	258	ALA	2.7
1	G	74	GLY	2.7
1	K	137	ILE	2.7



Mol	Chain	Res	Type	RSRZ
1	K	153	ILE	2.7
1	Ν	338	SER	2.7
1	G	267	PHE	2.7
1	L	7	ILE	2.7
1	F	82	ALA	2.7
1	Н	226	MET	2.7
1	Ι	64	GLY	2.7
1	0	21	LEU	2.6
1	J	153	ILE	2.6
1	В	9	GLY	2.6
1	С	97	VAL	2.6
1	Ι	125	ILE	2.6
1	D	148	GLY	2.6
1	Ι	137	ILE	2.6
1	K	306	LYS	2.6
1	G	275	LEU	2.6
1	F	124	VAL	2.6
1	G	3	VAL	2.6
1	J	125	ILE	2.5
1	0	229	LEU	2.5
1	G	34	VAL	2.5
1	В	154	SER	2.5
1	0	136	THR	2.5
1	J	3	VAL	2.5
1	L	118	ASP	2.5
1	Ν	124	VAL	2.5
1	0	167	ALA	2.5
1	С	153	ILE	2.5
1	L	116	HIS	2.5
1	J	146	TYR	2.4
1	K	328	LEU	2.4
1	D	332	VAL	2.4
1	А	312	ALA	2.4
1	Е	167	ALA	2.4
1	Н	107	PHE	2.4
1	С	123	LYS	2.4
1	0	126	ILE	2.4
1	L	80	ALA	2.4
1	J	85	GLU	2.4
1	С	117	LEU	2.4
1	Ι	32	VAL	2.4
1	0	98	ASP	2.3



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Mol	Chain	Res	Type	RSRZ
1	Κ	258	ALA	2.3
1	0	251	THR	2.3
1	В	127	SER	2.3
1	K	170	LEU	2.3
1	Κ	256	THR	2.3
1	G	75	ARG	2.3
1	С	70	THR	2.3
1	М	6	GLY	2.3
1	Ι	82	ALA	2.3
1	J	325	SER	2.3
1	J	99	VAL	2.3
1	М	70	THR	2.2
1	J	137	ILE	2.2
1	А	311	GLN	2.2
1	F	235	GLY	2.2
1	G	30	ALA	2.2
1	J	30	ALA	2.2
1	Κ	17	PHE	2.2
1	J	333	THR	2.2
1	В	130	ALA	2.2
1	D	94	ASP	2.2
1	F	92	TRP	2.2
1	В	149	SER	2.2
1	J	144	ASP	2.2
1	0	127	SER	2.1
1	0	143	ASP	2.1
1	М	46	LEU	2.1
1	Κ	130	ALA	2.1
1	С	99	VAL	2.1
1	Н	336	GLY	2.1
1	J	110	ALA	2.1
1	J	32	VAL	2.1
1	Κ	311	GLN	2.1
1	М	224	LEU	2.1
1	J	154	SER	2.1
1	F	135	ILE	2.1
1	J	264	ASN	2.1
1	Е	139	LEU	2.1
1	Ι	148	GLY	2.1
1	Н	91	PRO	2.1
1	0	118	ASP	2.1
1	L	139	LEU	2.0



Mol	Chain	Res	Type	RSRZ
1	Е	311	GLN	2.0
1	G	5	VAL	2.0
1	Ν	329	VAL	2.0
1	G	279	LEU	2.0
1	М	135	ILE	2.0
1	С	310	ASP	2.0
1	В	66	GLU	2.0
1	В	34	VAL	2.0
1	Ν	308	ILE	2.0
1	Ν	312	ALA	2.0
1	Р	255	SER	2.0
1	0	156	ALA	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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ² )	Q<0.9
3	EDO	D	402	4/4	0.71	0.31	29,39,39,40	0
2	NAD	0	401	44/44	0.84	0.26	46,59,75,76	0
2	NAD	Р	401	44/44	0.88	0.26	36,48,54,64	0
2	NAD	М	401	44/44	0.89	0.23	$43,\!51,\!56,\!61$	0
2	NAD	Ι	401	44/44	0.89	0.22	35,44,50,54	0
2	NAD	В	401	44/44	0.90	0.22	29,41,46,48	0
2	NAD	J	401	44/44	0.90	0.23	47,55,60,65	0
2	NAD	N	401	44/44	0.91	0.21	39,49,53,54	0
2	NAD	А	401	44/44	0.91	0.22	33,41,47,52	0
2	NAD	Е	401	44/44	0.91	0.21	33,41,48,50	0
2	NAD	Н	401	44/44	0.91	0.22	31,40,46,47	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ² )	Q<0.9
3	EDO	А	402	4/4	0.92	0.14	$29,\!35,\!37,\!38$	0
2	NAD	L	401	44/44	0.92	0.20	$35,\!46,\!51,\!57$	0
2	NAD	D	401	44/44	0.93	0.19	33,44,48,50	0
2	NAD	Κ	401	44/44	0.93	0.17	38,47,53,54	0
2	NAD	G	401	44/44	0.93	0.19	29,41,47,49	0
2	NAD	С	401	44/44	0.94	0.18	35,41,45,49	0
2	NAD	F	401	44/44	0.94	0.17	34,38,43,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



































# 6.5 Other polymers (i)

There are no such residues in this entry.

