



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:22 am BST

PDB ID : 3SXP  
Title : Crystal Structure of Helicobacter pylori ADP-L-glycero-D-manno-heptose-6-phosphatase (rfaD, HP0859)  
Authors : Shaik, M.M.; Zanotti, G.; Cendron, L.  
Deposited on : 2011-07-15  
Resolution : 2.55 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](mailto: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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

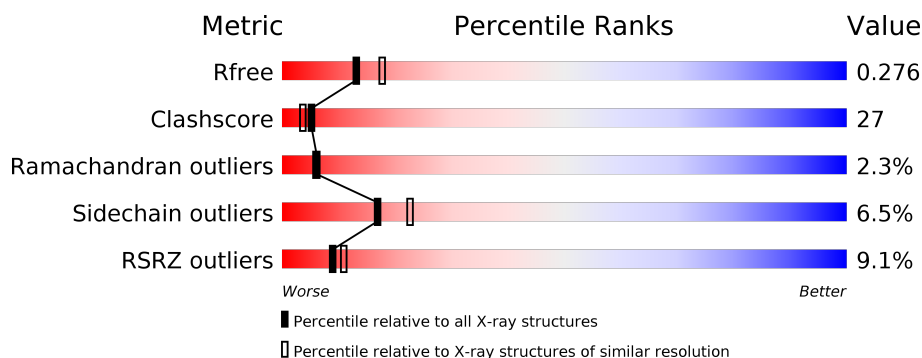
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	362	<div> <div>7%</div> <div> <div>43%</div> <div>38%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	362	<div> <div>4%</div> <div> <div>43%</div> <div>39%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	362	<div> <div>12%</div> <div> <div>43%</div> <div>39%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	362	<div> <div>8%</div> <div> <div>45%</div> <div>38%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	362	<div> <div>9%</div> <div> <div>45%</div> <div>36%</div> <div>•</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12913 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 ADP-L-glycero-D-mannoheptose-6-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2480	1596	416	460	8			
1	B	311	Total	C	N	O	S	0	0	0
			2489	1601	418	462	8			
1	C	310	Total	C	N	O	S	0	0	0
			2480	1596	416	460	8			
1	D	314	Total	C	N	O	S	0	0	0
			2519	1623	422	466	8			
1	E	310	Total	C	N	O	S	0	0	0
			2480	1596	416	460	8			

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLU	GLY	ENGINEERED MUTATION	UNP B5Z7L9
A	331	LYS	-	EXPRESSION TAG	UNP B5Z7L9
A	332	GLY	-	EXPRESSION TAG	UNP B5Z7L9
A	333	GLU	-	EXPRESSION TAG	UNP B5Z7L9
A	334	LEU	-	EXPRESSION TAG	UNP B5Z7L9
A	335	ASN	-	EXPRESSION TAG	UNP B5Z7L9
A	336	SER	-	EXPRESSION TAG	UNP B5Z7L9
A	337	LYS	-	EXPRESSION TAG	UNP B5Z7L9
A	338	LEU	-	EXPRESSION TAG	UNP B5Z7L9
A	339	GLU	-	EXPRESSION TAG	UNP B5Z7L9
A	340	GLY	-	EXPRESSION TAG	UNP B5Z7L9
A	341	LYS	-	EXPRESSION TAG	UNP B5Z7L9
A	342	PRO	-	EXPRESSION TAG	UNP B5Z7L9
A	343	ILE	-	EXPRESSION TAG	UNP B5Z7L9
A	344	PRO	-	EXPRESSION TAG	UNP B5Z7L9
A	345	ASN	-	EXPRESSION TAG	UNP B5Z7L9
A	346	LEU	-	EXPRESSION TAG	UNP B5Z7L9
A	347	LEU	-	EXPRESSION TAG	UNP B5Z7L9
A	348	GLY	-	EXPRESSION TAG	UNP B5Z7L9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	349	LEU	-	EXPRESSION TAG	UNP B5Z7L9
A	350	ASP	-	EXPRESSION TAG	UNP B5Z7L9
A	351	SER	-	EXPRESSION TAG	UNP B5Z7L9
A	352	THR	-	EXPRESSION TAG	UNP B5Z7L9
A	353	ARG	-	EXPRESSION TAG	UNP B5Z7L9
A	354	THR	-	EXPRESSION TAG	UNP B5Z7L9
A	355	GLY	-	EXPRESSION TAG	UNP B5Z7L9
A	356	HIS	-	EXPRESSION TAG	UNP B5Z7L9
A	357	HIS	-	EXPRESSION TAG	UNP B5Z7L9
A	358	HIS	-	EXPRESSION TAG	UNP B5Z7L9
A	359	HIS	-	EXPRESSION TAG	UNP B5Z7L9
A	360	HIS	-	EXPRESSION TAG	UNP B5Z7L9
A	361	HIS	-	EXPRESSION TAG	UNP B5Z7L9
A	362	HIS	-	EXPRESSION TAG	UNP B5Z7L9
B	7	GLU	GLY	ENGINEERED MUTATION	UNP B5Z7L9
B	331	LYS	-	EXPRESSION TAG	UNP B5Z7L9
B	332	GLY	-	EXPRESSION TAG	UNP B5Z7L9
B	333	GLU	-	EXPRESSION TAG	UNP B5Z7L9
B	334	LEU	-	EXPRESSION TAG	UNP B5Z7L9
B	335	ASN	-	EXPRESSION TAG	UNP B5Z7L9
B	336	SER	-	EXPRESSION TAG	UNP B5Z7L9
B	337	LYS	-	EXPRESSION TAG	UNP B5Z7L9
B	338	LEU	-	EXPRESSION TAG	UNP B5Z7L9
B	339	GLU	-	EXPRESSION TAG	UNP B5Z7L9
B	340	GLY	-	EXPRESSION TAG	UNP B5Z7L9
B	341	LYS	-	EXPRESSION TAG	UNP B5Z7L9
B	342	PRO	-	EXPRESSION TAG	UNP B5Z7L9
B	343	ILE	-	EXPRESSION TAG	UNP B5Z7L9
B	344	PRO	-	EXPRESSION TAG	UNP B5Z7L9
B	345	ASN	-	EXPRESSION TAG	UNP B5Z7L9
B	346	LEU	-	EXPRESSION TAG	UNP B5Z7L9
B	347	LEU	-	EXPRESSION TAG	UNP B5Z7L9
B	348	GLY	-	EXPRESSION TAG	UNP B5Z7L9
B	349	LEU	-	EXPRESSION TAG	UNP B5Z7L9
B	350	ASP	-	EXPRESSION TAG	UNP B5Z7L9
B	351	SER	-	EXPRESSION TAG	UNP B5Z7L9
B	352	THR	-	EXPRESSION TAG	UNP B5Z7L9
B	353	ARG	-	EXPRESSION TAG	UNP B5Z7L9
B	354	THR	-	EXPRESSION TAG	UNP B5Z7L9
B	355	GLY	-	EXPRESSION TAG	UNP B5Z7L9
B	356	HIS	-	EXPRESSION TAG	UNP B5Z7L9
B	357	HIS	-	EXPRESSION TAG	UNP B5Z7L9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	358	HIS	-	EXPRESSION TAG	UNP B5Z7L9
B	359	HIS	-	EXPRESSION TAG	UNP B5Z7L9
B	360	HIS	-	EXPRESSION TAG	UNP B5Z7L9
B	361	HIS	-	EXPRESSION TAG	UNP B5Z7L9
B	362	HIS	-	EXPRESSION TAG	UNP B5Z7L9
C	7	GLU	GLY	ENGINEERED MUTATION	UNP B5Z7L9
C	331	LYS	-	EXPRESSION TAG	UNP B5Z7L9
C	332	GLY	-	EXPRESSION TAG	UNP B5Z7L9
C	333	GLU	-	EXPRESSION TAG	UNP B5Z7L9
C	334	LEU	-	EXPRESSION TAG	UNP B5Z7L9
C	335	ASN	-	EXPRESSION TAG	UNP B5Z7L9
C	336	SER	-	EXPRESSION TAG	UNP B5Z7L9
C	337	LYS	-	EXPRESSION TAG	UNP B5Z7L9
C	338	LEU	-	EXPRESSION TAG	UNP B5Z7L9
C	339	GLU	-	EXPRESSION TAG	UNP B5Z7L9
C	340	GLY	-	EXPRESSION TAG	UNP B5Z7L9
C	341	LYS	-	EXPRESSION TAG	UNP B5Z7L9
C	342	PRO	-	EXPRESSION TAG	UNP B5Z7L9
C	343	ILE	-	EXPRESSION TAG	UNP B5Z7L9
C	344	PRO	-	EXPRESSION TAG	UNP B5Z7L9
C	345	ASN	-	EXPRESSION TAG	UNP B5Z7L9
C	346	LEU	-	EXPRESSION TAG	UNP B5Z7L9
C	347	LEU	-	EXPRESSION TAG	UNP B5Z7L9
C	348	GLY	-	EXPRESSION TAG	UNP B5Z7L9
C	349	LEU	-	EXPRESSION TAG	UNP B5Z7L9
C	350	ASP	-	EXPRESSION TAG	UNP B5Z7L9
C	351	SER	-	EXPRESSION TAG	UNP B5Z7L9
C	352	THR	-	EXPRESSION TAG	UNP B5Z7L9
C	353	ARG	-	EXPRESSION TAG	UNP B5Z7L9
C	354	THR	-	EXPRESSION TAG	UNP B5Z7L9
C	355	GLY	-	EXPRESSION TAG	UNP B5Z7L9
C	356	HIS	-	EXPRESSION TAG	UNP B5Z7L9
C	357	HIS	-	EXPRESSION TAG	UNP B5Z7L9
C	358	HIS	-	EXPRESSION TAG	UNP B5Z7L9
C	359	HIS	-	EXPRESSION TAG	UNP B5Z7L9
C	360	HIS	-	EXPRESSION TAG	UNP B5Z7L9
C	361	HIS	-	EXPRESSION TAG	UNP B5Z7L9
C	362	HIS	-	EXPRESSION TAG	UNP B5Z7L9
D	7	GLU	GLY	ENGINEERED MUTATION	UNP B5Z7L9
D	331	LYS	-	EXPRESSION TAG	UNP B5Z7L9
D	332	GLY	-	EXPRESSION TAG	UNP B5Z7L9
D	333	GLU	-	EXPRESSION TAG	UNP B5Z7L9

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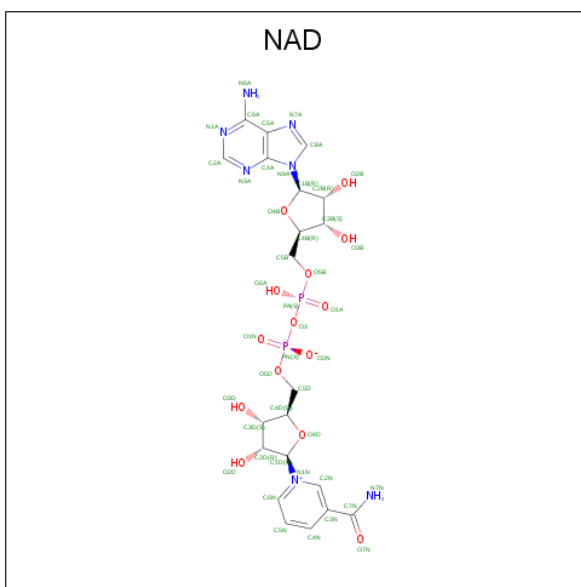
Chain	Residue	Modelled	Actual	Comment	Reference
D	334	LEU	-	EXPRESSION TAG	UNP B5Z7L9
D	335	ASN	-	EXPRESSION TAG	UNP B5Z7L9
D	336	SER	-	EXPRESSION TAG	UNP B5Z7L9
D	337	LYS	-	EXPRESSION TAG	UNP B5Z7L9
D	338	LEU	-	EXPRESSION TAG	UNP B5Z7L9
D	339	GLU	-	EXPRESSION TAG	UNP B5Z7L9
D	340	GLY	-	EXPRESSION TAG	UNP B5Z7L9
D	341	LYS	-	EXPRESSION TAG	UNP B5Z7L9
D	342	PRO	-	EXPRESSION TAG	UNP B5Z7L9
D	343	ILE	-	EXPRESSION TAG	UNP B5Z7L9
D	344	PRO	-	EXPRESSION TAG	UNP B5Z7L9
D	345	ASN	-	EXPRESSION TAG	UNP B5Z7L9
D	346	LEU	-	EXPRESSION TAG	UNP B5Z7L9
D	347	LEU	-	EXPRESSION TAG	UNP B5Z7L9
D	348	GLY	-	EXPRESSION TAG	UNP B5Z7L9
D	349	LEU	-	EXPRESSION TAG	UNP B5Z7L9
D	350	ASP	-	EXPRESSION TAG	UNP B5Z7L9
D	351	SER	-	EXPRESSION TAG	UNP B5Z7L9
D	352	THR	-	EXPRESSION TAG	UNP B5Z7L9
D	353	ARG	-	EXPRESSION TAG	UNP B5Z7L9
D	354	THR	-	EXPRESSION TAG	UNP B5Z7L9
D	355	GLY	-	EXPRESSION TAG	UNP B5Z7L9
D	356	HIS	-	EXPRESSION TAG	UNP B5Z7L9
D	357	HIS	-	EXPRESSION TAG	UNP B5Z7L9
D	358	HIS	-	EXPRESSION TAG	UNP B5Z7L9
D	359	HIS	-	EXPRESSION TAG	UNP B5Z7L9
D	360	HIS	-	EXPRESSION TAG	UNP B5Z7L9
D	361	HIS	-	EXPRESSION TAG	UNP B5Z7L9
D	362	HIS	-	EXPRESSION TAG	UNP B5Z7L9
E	7	GLU	GLY	ENGINEERED MUTATION	UNP B5Z7L9
E	331	LYS	-	EXPRESSION TAG	UNP B5Z7L9
E	332	GLY	-	EXPRESSION TAG	UNP B5Z7L9
E	333	GLU	-	EXPRESSION TAG	UNP B5Z7L9
E	334	LEU	-	EXPRESSION TAG	UNP B5Z7L9
E	335	ASN	-	EXPRESSION TAG	UNP B5Z7L9
E	336	SER	-	EXPRESSION TAG	UNP B5Z7L9
E	337	LYS	-	EXPRESSION TAG	UNP B5Z7L9
E	338	LEU	-	EXPRESSION TAG	UNP B5Z7L9
E	339	GLU	-	EXPRESSION TAG	UNP B5Z7L9
E	340	GLY	-	EXPRESSION TAG	UNP B5Z7L9
E	341	LYS	-	EXPRESSION TAG	UNP B5Z7L9
E	342	PRO	-	EXPRESSION TAG	UNP B5Z7L9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	ILE	-	EXPRESSION TAG	UNP B5Z7L9
E	344	PRO	-	EXPRESSION TAG	UNP B5Z7L9
E	345	ASN	-	EXPRESSION TAG	UNP B5Z7L9
E	346	LEU	-	EXPRESSION TAG	UNP B5Z7L9
E	347	LEU	-	EXPRESSION TAG	UNP B5Z7L9
E	348	GLY	-	EXPRESSION TAG	UNP B5Z7L9
E	349	LEU	-	EXPRESSION TAG	UNP B5Z7L9
E	350	ASP	-	EXPRESSION TAG	UNP B5Z7L9
E	351	SER	-	EXPRESSION TAG	UNP B5Z7L9
E	352	THR	-	EXPRESSION TAG	UNP B5Z7L9
E	353	ARG	-	EXPRESSION TAG	UNP B5Z7L9
E	354	THR	-	EXPRESSION TAG	UNP B5Z7L9
E	355	GLY	-	EXPRESSION TAG	UNP B5Z7L9
E	356	HIS	-	EXPRESSION TAG	UNP B5Z7L9
E	357	HIS	-	EXPRESSION TAG	UNP B5Z7L9
E	358	HIS	-	EXPRESSION TAG	UNP B5Z7L9
E	359	HIS	-	EXPRESSION TAG	UNP B5Z7L9
E	360	HIS	-	EXPRESSION TAG	UNP B5Z7L9
E	361	HIS	-	EXPRESSION TAG	UNP B5Z7L9
E	362	HIS	-	EXPRESSION TAG	UNP B5Z7L9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$ ).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	56	Total	O	0	0
			56	56		
3	C	36	Total	O	0	0
			36	36		
3	D	43	Total	O	0	0
			43	43		
3	E	42	Total	O	0	0
			42	42		

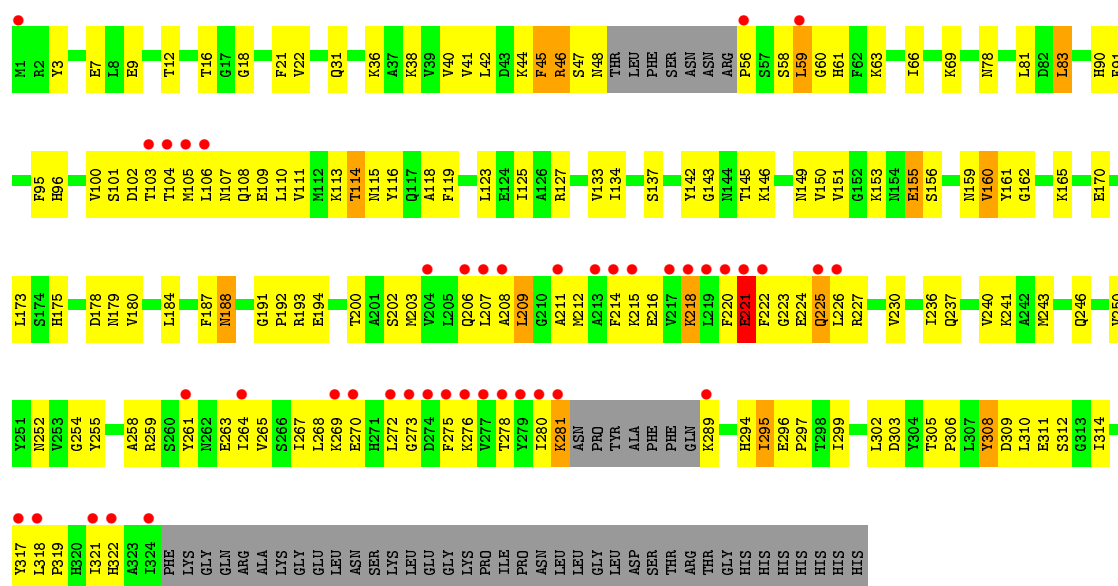




PHE  
LYS  
GLY  
GLN  
ARG  
ALA  
LYS  
GLY  
LEU  
ASN  
SER  
LYS  
LEU  
GLY  
LYS  
PRO  
TLE  
PRO  
ASN  
LEU  
LEU  
GLY  
LEU  
ASP  
SER  
THR  
THR  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS

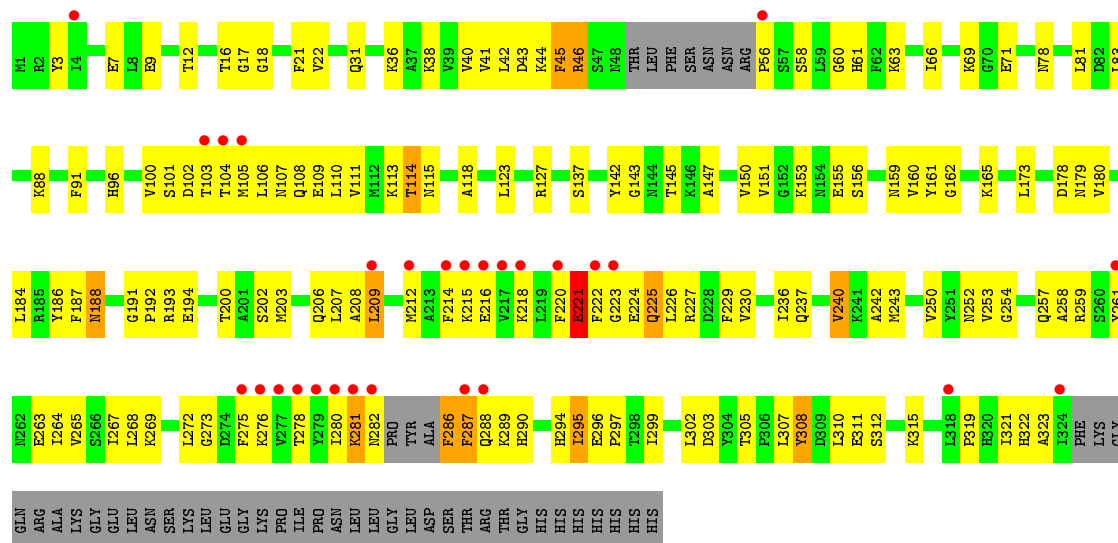
• Molecule 1: ADP-L-glycero-D-mannoheptose-6-epimerase

Chain C: 12% 43% 39% 14%



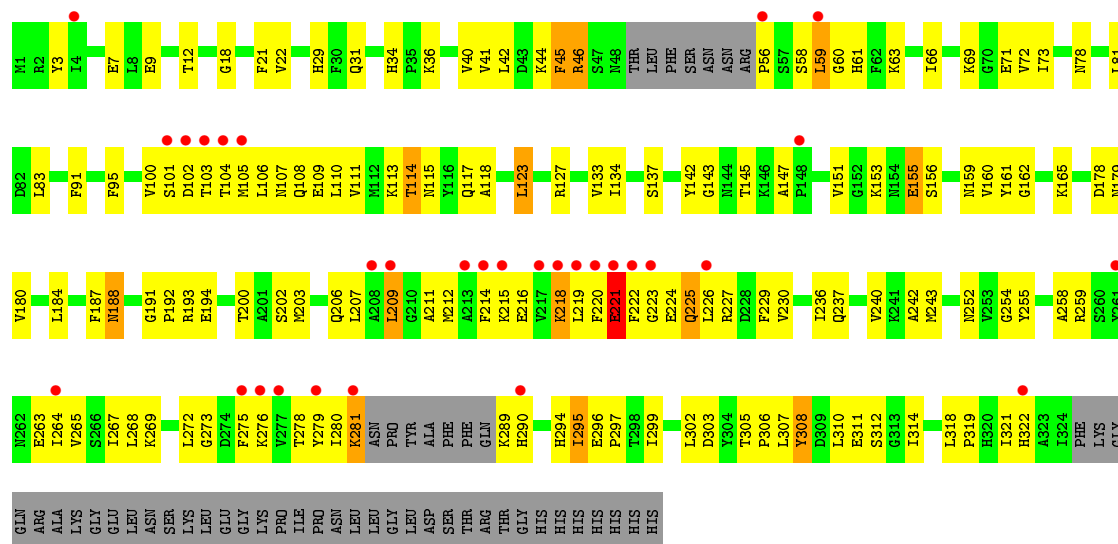
• Molecule 1: ADP-L-glycero-D-mannoheptose-6-epimerase

Chain D: 8% 45% 38% 13%



• Molecule 1: ADP-L-glycero-D-mannoheptose-6-epimerase

Chain E: 9% 45% 36% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.94Å 106.77Å 152.22Å 90.00° 108.35° 90.00°	Depositor
Resolution (Å)	53.39 – 2.55 53.38 – 2.55	Depositor EDS
% Data completeness (in resolution range)	85.6 (53.39-2.55) 85.6 (53.38-2.55)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.55Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.239 , 0.279 0.238 , 0.276	Depositor DCC
$R_{free}$ test set	2808 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 76.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.47	0/2532	0.66	1/3415 (0.0%)
1	B	0.47	0/2541	0.66	0/3427
1	C	0.48	0/2532	0.66	0/3415
1	D	0.47	0/2573	0.67	1/3470 (0.0%)
1	E	0.49	0/2532	0.67	0/3415
All	All	0.48	0/12710	0.66	2/17142 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	307	LEU	N-CA-C	-5.21	96.93	111.00
1	A	294	HIS	N-CA-C	-5.01	97.48	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	2480	0	2469	136	0
1	B	2489	0	2477	136	0
1	C	2480	0	2469	138	0
1	D	2519	0	2501	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2480	0	2469	134	0
2	A	44	0	26	3	0
2	B	44	0	26	6	0
2	C	44	0	26	4	0
2	D	44	0	25	4	0
2	E	44	0	26	5	0
3	A	68	0	0	7	0
3	B	56	0	0	4	0
3	C	36	0	0	5	0
3	D	43	0	0	3	0
3	E	42	0	0	3	0
All	All	12913	0	12514	671	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 27.

All (671) 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:C:59:LEU:HD21	1:C:101:SER:CB	1.61	1.31
1:B:59:LEU:CD2	1:B:101:SER:HB3	1.63	1.29
1:B:59:LEU:HD21	1:B:101:SER:CB	1.75	1.17
1:C:59:LEU:HD21	1:C:101:SER:HB3	1.28	1.14
1:C:59:LEU:HD21	1:C:101:SER:HB2	1.39	1.04
1:C:31:GLN:NE2	1:C:69:LYS:H	1.59	0.99
1:A:31:GLN:NE2	1:A:69:LYS:H	1.63	0.95
1:B:31:GLN:NE2	1:B:69:LYS:H	1.64	0.95
1:E:31:GLN:NE2	1:E:69:LYS:H	1.66	0.94
1:D:31:GLN:NE2	1:D:69:LYS:H	1.67	0.93
1:A:31:GLN:HE22	1:A:69:LYS:H	0.91	0.91
1:C:59:LEU:CD2	1:C:101:SER:HB3	2.01	0.90
1:C:31:GLN:HE22	1:C:69:LYS:N	1.69	0.89
1:C:59:LEU:CD2	1:C:101:SER:CB	2.51	0.88
1:B:59:LEU:HD23	1:B:59:LEU:N	1.89	0.88
1:E:31:GLN:HE22	1:E:69:LYS:N	1.72	0.87
1:B:31:GLN:HE22	1:B:69:LYS:N	1.72	0.87
1:D:212:MET:HE1	1:D:322:HIS:HA	1.54	0.87
1:E:212:MET:HE1	1:E:322:HIS:HA	1.56	0.87
1:B:237:GLN:HE22	1:B:305:THR:H	1.22	0.86
1:B:31:GLN:HE22	1:B:69:LYS:H	0.87	0.86
1:A:159:ASN:ND2	1:A:161:TYR:HB3	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:HIS:HD2	1:C:63:LYS:H	1.23	0.86
1:E:61:HIS:HD2	1:E:63:LYS:H	1.23	0.85
1:D:31:GLN:HE22	1:D:69:LYS:N	1.74	0.85
1:D:159:ASN:ND2	1:D:161:TYR:HB3	1.92	0.85
1:E:237:GLN:HE22	1:E:305:THR:H	1.25	0.84
1:B:61:HIS:HD2	1:B:63:LYS:H	1.22	0.84
1:A:237:GLN:HE22	1:A:305:THR:H	1.26	0.84
1:C:212:MET:HE1	1:C:322:HIS:HA	1.59	0.83
1:D:31:GLN:HE22	1:D:69:LYS:H	0.89	0.83
1:A:31:GLN:HE22	1:A:69:LYS:N	1.75	0.83
1:E:100:VAL:H	1:E:115:ASN:HD21	1.26	0.82
1:E:159:ASN:ND2	1:E:161:TYR:HB3	1.94	0.82
1:E:296:GLU:HB2	1:E:297:PRO:HD3	1.62	0.81
1:E:31:GLN:HE22	1:E:69:LYS:H	0.87	0.81
1:C:237:GLN:HE22	1:C:305:THR:H	1.26	0.80
1:A:100:VAL:H	1:A:115:ASN:HD21	1.28	0.80
1:B:100:VAL:H	1:B:115:ASN:HD21	1.26	0.79
1:B:159:ASN:ND2	1:B:161:TYR:HB3	1.97	0.79
1:C:18:GLY:HA3	1:C:41:VAL:HG13	1.64	0.79
1:D:100:VAL:H	1:D:115:ASN:HD21	1.27	0.79
1:D:237:GLN:HE22	1:D:305:THR:H	1.27	0.79
1:E:18:GLY:HA3	1:E:41:VAL:HG13	1.66	0.78
1:A:18:GLY:HA3	1:A:41:VAL:HG13	1.66	0.78
1:C:159:ASN:ND2	1:C:161:TYR:HB3	1.98	0.78
1:A:308:TYR:HA	1:A:312:SER:HB2	1.66	0.77
1:A:61:HIS:HD2	1:A:63:LYS:H	1.33	0.76
1:C:31:GLN:HE22	1:C:69:LYS:H	0.84	0.75
1:C:100:VAL:H	1:C:115:ASN:HD21	1.33	0.75
1:A:59:LEU:HD11	1:A:101:SER:HB2	1.68	0.74
1:D:296:GLU:HB2	1:D:297:PRO:HD3	1.68	0.74
1:C:308:TYR:HA	1:C:312:SER:HB2	1.68	0.74
1:B:308:TYR:HA	1:B:312:SER:HB2	1.70	0.74
1:E:308:TYR:HA	1:E:312:SER:HB2	1.70	0.74
1:D:308:TYR:HA	1:D:312:SER:HB2	1.70	0.73
1:A:34:HIS:HE1	3:A:403:HOH:O	1.71	0.73
1:C:146:LYS:HE2	3:C:393:HOH:O	1.89	0.72
1:D:288:GLN:N	1:D:289:LYS:HZ3	1.88	0.72
1:C:296:GLU:HB2	1:C:297:PRO:HD3	1.70	0.72
1:D:61:HIS:HD2	1:D:63:LYS:H	1.36	0.72
1:B:59:LEU:H	1:B:59:LEU:HD23	1.55	0.72
1:D:221:GLU:HA	1:D:281:LYS:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:GLY:HA3	1:D:41:VAL:HG13	1.72	0.71
1:B:48:ASN:H	1:D:107:ASN:ND2	1.90	0.70
1:E:104:THR:O	1:E:106:LEU:HG	1.90	0.70
1:E:61:HIS:CD2	1:E:63:LYS:H	2.08	0.70
1:E:153:LYS:HE2	1:E:153:LYS:HA	1.74	0.70
1:B:9:GLU:HG3	1:B:36:LYS:HD3	1.74	0.70
1:B:59:LEU:HD21	1:B:101:SER:HB3	0.79	0.69
1:D:236:ILE:O	1:D:240:VAL:HG12	1.93	0.69
1:A:296:GLU:HB2	1:A:297:PRO:HD3	1.74	0.69
1:B:296:GLU:HB2	1:B:297:PRO:HD3	1.74	0.69
1:C:221:GLU:HA	1:C:281:LYS:HE2	1.74	0.69
1:D:22:VAL:HG22	2:D:2401:NAD:H51N	1.74	0.69
1:E:240:VAL:O	1:E:243:MET:HG2	1.92	0.69
1:E:221:GLU:HA	1:E:281:LYS:HE2	1.73	0.69
1:C:236:ILE:O	1:C:240:VAL:HG12	1.93	0.68
1:E:237:GLN:NE2	1:E:305:THR:H	1.92	0.68
1:A:9:GLU:HG3	1:A:36:LYS:HD3	1.75	0.68
1:B:61:HIS:CD2	1:B:63:LYS:H	2.09	0.68
1:D:104:THR:O	1:D:106:LEU:HG	1.93	0.68
1:B:221:GLU:HA	1:B:281:LYS:HE2	1.76	0.68
1:A:127:ARG:HD2	1:A:178:ASP:HB3	1.75	0.67
1:B:47:SER:HA	1:D:107:ASN:HD21	1.56	0.67
1:C:61:HIS:CD2	1:C:63:LYS:H	2.10	0.67
1:E:29:HIS:HE1	3:E:376:HOH:O	1.77	0.66
1:C:127:ARG:HD2	1:C:178:ASP:HB3	1.76	0.66
1:E:59:LEU:HD11	1:E:101:SER:HB2	1.77	0.66
1:A:240:VAL:O	1:A:243:MET:HG2	1.96	0.66
1:A:61:HIS:CD2	1:A:63:LYS:H	2.14	0.66
1:B:237:GLN:NE2	1:B:305:THR:H	1.92	0.66
1:D:323:ALA:HB2	3:D:400:HOH:O	1.96	0.65
1:B:59:LEU:CD2	1:B:101:SER:CB	2.50	0.65
1:D:257:GLN:HB2	3:D:384:HOH:O	1.95	0.65
1:B:18:GLY:HA3	1:B:41:VAL:HG13	1.78	0.65
1:C:237:GLN:NE2	1:C:305:THR:H	1.95	0.65
1:A:71:GLU:HA	3:A:424:HOH:O	1.97	0.65
1:B:102:ASP:O	1:B:105:MET:HG2	1.98	0.64
1:B:104:THR:O	1:B:106:LEU:HG	1.97	0.64
1:D:280:ILE:C	1:D:281:LYS:HD2	2.17	0.64
1:E:179:ASN:ND2	1:E:180:VAL:H	1.95	0.64
1:E:103:THR:HB	1:E:200:THR:CG2	2.28	0.64
1:B:103:THR:HB	1:B:200:THR:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:HA	1:A:281:LYS:HE2	1.78	0.64
1:D:102:ASP:O	1:D:105:MET:HG2	1.97	0.64
1:C:104:THR:O	1:C:106:LEU:HG	1.98	0.63
1:E:258:ALA:O	1:E:259:ARG:HD2	1.99	0.63
1:D:9:GLU:HG3	1:D:36:LYS:HD3	1.79	0.63
1:A:289:LYS:N	1:A:289:LYS:HD2	2.14	0.63
1:C:102:ASP:O	1:C:105:MET:HG2	1.99	0.63
1:E:236:ILE:O	1:E:240:VAL:HG12	1.97	0.63
1:A:102:ASP:O	1:A:105:MET:HG2	1.99	0.63
1:A:159:ASN:HD21	1:A:161:TYR:HB3	1.64	0.63
1:C:165:LYS:NZ	2:C:2403:NAD:O3D	2.31	0.62
1:A:103:THR:HB	1:A:200:THR:CG2	2.29	0.62
1:B:288:GLN:N	1:B:289:LYS:HZ3	1.97	0.62
1:C:109:GLU:O	1:C:113:LYS:HG2	2.00	0.62
1:A:237:GLN:NE2	1:A:305:THR:H	1.95	0.62
1:E:191:GLY:O	1:E:194:GLU:HG2	1.99	0.62
1:C:22:VAL:CG2	2:C:2403:NAD:H51N	2.29	0.62
1:D:103:THR:HB	1:D:200:THR:CG2	2.29	0.62
1:C:151:VAL:HG23	1:C:252:ASN:ND2	2.15	0.62
1:B:220:PHE:HA	1:B:280:ILE:HG23	1.81	0.62
1:A:104:THR:O	1:A:106:LEU:HG	2.00	0.61
1:D:44:LYS:O	1:D:45:PHE:HB2	1.99	0.61
1:D:237:GLN:NE2	1:D:305:THR:H	1.97	0.61
1:B:170:GLU:OE1	1:E:69:LYS:HD2	1.99	0.61
1:B:212:MET:HE1	1:B:322:HIS:HA	1.82	0.61
1:D:61:HIS:CD2	1:D:63:LYS:H	2.18	0.61
1:C:7:GLU:HG3	1:C:36:LYS:HD2	1.82	0.61
1:A:264:ILE:O	1:A:268:LEU:HB2	2.01	0.61
1:E:34:HIS:HE1	3:E:376:HOH:O	1.84	0.61
1:E:202:SER:O	1:E:206:GLN:HG2	2.01	0.61
1:C:191:GLY:O	1:C:194:GLU:HG2	2.00	0.60
1:C:264:ILE:O	1:C:268:LEU:HB2	2.01	0.60
1:E:22:VAL:HG22	2:E:2403:NAD:H51N	1.82	0.60
1:C:44:LYS:O	1:C:45:PHE:HB2	2.01	0.60
1:A:107:ASN:OD1	1:A:110:LEU:HD13	2.01	0.60
1:C:103:THR:HG23	1:C:104:THR:H	1.67	0.60
1:C:149:ASN:HA	3:C:382:HOH:O	2.01	0.60
1:E:137:SER:O	2:E:2403:NAD:H6N	2.01	0.60
1:A:153:LYS:HE2	1:A:153:LYS:HA	1.83	0.60
1:A:212:MET:HE1	1:A:322:HIS:HA	1.83	0.60
1:C:103:THR:HB	1:C:200:THR:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLU:CG	1:C:36:LYS:HD2	2.32	0.60
1:D:22:VAL:CG2	2:D:2401:NAD:H51N	2.32	0.60
1:A:59:LEU:HD11	1:A:101:SER:CB	2.32	0.60
1:C:220:PHE:HA	1:C:280:ILE:HG23	1.83	0.60
1:D:289:LYS:HD2	1:D:289:LYS:N	2.17	0.60
1:A:103:THR:HB	1:A:200:THR:HG21	1.84	0.60
1:A:29:HIS:HE1	3:A:403:HOH:O	1.84	0.60
1:B:113:LYS:HD2	3:B:401:HOH:O	2.01	0.60
1:C:103:THR:HG23	1:C:104:THR:N	2.17	0.60
1:E:264:ILE:O	1:E:268:LEU:HB2	2.02	0.60
1:B:188:ASN:ND2	3:B:390:HOH:O	2.35	0.60
1:B:216:GLU:HG3	1:B:276:LYS:HB3	1.84	0.60
1:D:281:LYS:N	1:D:281:LYS:HD2	2.17	0.60
1:A:236:ILE:O	1:A:240:VAL:HG12	2.02	0.59
1:C:223:GLY:HA2	1:C:225:GLN:OE1	2.01	0.59
1:B:240:VAL:O	1:B:243:MET:HG2	2.02	0.59
1:D:287:PHE:C	1:D:289:LYS:HZ3	2.05	0.59
1:A:105:MET:HG3	1:A:105:MET:O	2.02	0.59
1:E:187:PHE:O	1:E:230:VAL:HG12	2.02	0.59
1:A:263:GLU:O	1:A:267:ILE:HG13	2.02	0.59
1:A:85:ARG:HD3	3:A:430:HOH:O	2.03	0.59
1:A:191:GLY:O	1:A:194:GLU:HG2	2.02	0.59
1:E:78:ASN:ND2	1:E:118:ALA:HB2	2.18	0.59
1:A:216:GLU:HG3	1:A:276:LYS:HB3	1.85	0.58
1:A:220:PHE:HA	1:A:280:ILE:HG23	1.85	0.58
1:B:109:GLU:O	1:B:113:LYS:HG2	2.03	0.58
1:E:127:ARG:HD2	1:E:178:ASP:HB3	1.85	0.58
2:B:2401:NAD:O3D	3:B:403:HOH:O	2.04	0.58
1:C:78:ASN:ND2	1:C:118:ALA:HB2	2.18	0.58
1:D:220:PHE:HA	1:D:280:ILE:HG23	1.84	0.58
1:B:179:ASN:ND2	1:B:180:VAL:H	2.02	0.58
1:C:47:SER:HA	1:E:107:ASN:HD21	1.66	0.58
1:C:267:ILE:HD13	1:C:311:GLU:HG3	1.85	0.58
1:D:159:ASN:HD22	1:D:161:TYR:HB3	1.68	0.58
1:A:22:VAL:HG22	2:A:2402:NAD:H51N	1.85	0.58
1:A:78:ASN:ND2	1:A:118:ALA:HB2	2.18	0.58
1:B:59:LEU:CD2	1:B:59:LEU:N	2.61	0.58
1:C:263:GLU:O	1:C:267:ILE:HG13	2.03	0.58
1:D:153:LYS:HA	1:D:153:LYS:HE2	1.85	0.58
1:E:220:PHE:HA	1:E:280:ILE:HG23	1.86	0.58
1:B:191:GLY:O	1:B:194:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ASN:OD1	1:D:110:LEU:HD13	2.03	0.58
1:A:202:SER:O	1:A:206:GLN:HG2	2.04	0.58
1:B:236:ILE:O	1:B:240:VAL:HG12	2.03	0.58
1:D:192:PRO:O	1:D:193:ARG:HB2	2.03	0.58
1:D:240:VAL:O	1:D:243:MET:HG2	2.03	0.58
1:C:216:GLU:HG3	1:C:276:LYS:HB3	1.86	0.58
1:A:7:GLU:CG	1:A:36:LYS:HD2	2.34	0.57
1:D:159:ASN:ND2	1:D:162:GLY:H	2.00	0.57
1:E:103:THR:HB	1:E:200:THR:HG21	1.84	0.57
1:C:46:ARG:HA	1:C:58:SER:O	2.03	0.57
1:E:103:THR:HG23	1:E:104:THR:H	1.68	0.57
1:A:44:LYS:O	1:A:45:PHE:HB2	2.03	0.57
1:A:7:GLU:HG3	1:A:36:LYS:HD2	1.87	0.57
1:B:103:THR:HG23	1:B:104:THR:H	1.70	0.57
1:C:280:ILE:C	1:C:281:LYS:HD2	2.25	0.57
1:B:159:ASN:HD21	1:B:161:TYR:HB3	1.69	0.57
1:D:46:ARG:HA	1:D:58:SER:O	2.04	0.57
1:B:22:VAL:HG22	2:B:2401:NAD:H51N	1.86	0.57
1:D:202:SER:O	1:D:206:GLN:HG2	2.04	0.57
1:D:258:ALA:O	1:D:259:ARG:HD2	2.04	0.57
1:B:159:ASN:ND2	1:B:162:GLY:H	2.03	0.57
1:C:159:ASN:ND2	1:C:162:GLY:H	2.02	0.57
1:E:44:LYS:O	1:E:45:PHE:HB2	2.03	0.57
1:A:247:LYS:HD3	3:A:426:HOH:O	2.02	0.57
1:B:103:THR:HG23	1:B:104:THR:N	2.19	0.57
1:D:103:THR:HG23	1:D:104:THR:H	1.70	0.57
1:A:280:ILE:C	1:A:281:LYS:HD2	2.25	0.57
1:C:153:LYS:HA	1:C:153:LYS:HE2	1.86	0.57
1:A:46:ARG:HA	1:A:58:SER:O	2.05	0.57
1:D:103:THR:HG23	1:D:104:THR:N	2.20	0.56
1:E:103:THR:HG23	1:E:104:THR:N	2.20	0.56
1:B:127:ARG:HD2	1:B:178:ASP:HB3	1.87	0.56
1:B:20:GLY:HA3	2:B:2401:NAD:H52A	1.86	0.56
1:E:102:ASP:O	1:E:105:MET:HG2	2.04	0.56
1:E:289:LYS:N	1:E:289:LYS:HD2	2.19	0.56
1:E:9:GLU:HG3	1:E:36:LYS:HD3	1.86	0.56
1:C:269:LYS:HA	1:C:273:GLY:O	2.05	0.56
1:E:46:ARG:HB2	1:E:60:GLY:O	2.06	0.56
1:C:187:PHE:O	1:C:230:VAL:HG12	2.06	0.56
1:A:109:GLU:O	1:A:113:LYS:HG2	2.04	0.56
1:A:187:PHE:O	1:A:230:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLY:H	1:C:295:ILE:HD11	1.71	0.56
1:D:286:PHE:C	1:D:288:GLN:H	2.09	0.56
1:E:203:MET:O	1:E:207:LEU:HG	2.05	0.56
1:C:46:ARG:HB2	1:C:60:GLY:O	2.06	0.56
1:D:179:ASN:ND2	1:D:180:VAL:H	2.04	0.56
1:D:127:ARG:HD2	1:D:178:ASP:HB3	1.87	0.56
1:E:108:GLN:HG3	1:E:160:VAL:CG1	2.36	0.56
1:E:109:GLU:O	1:E:113:LYS:HG2	2.06	0.56
1:A:159:ASN:HD22	1:A:161:TYR:HB3	1.71	0.55
1:B:105:MET:O	1:B:105:MET:HG3	2.06	0.55
1:B:103:THR:HB	1:B:200:THR:HG21	1.86	0.55
1:B:187:PHE:O	1:B:230:VAL:HG12	2.07	0.55
1:C:22:VAL:HG22	2:C:2403:NAD:H51N	1.87	0.55
1:C:240:VAL:O	1:C:243:MET:HG2	2.04	0.55
1:E:159:ASN:HD21	1:E:161:TYR:HB3	1.70	0.55
1:E:46:ARG:HA	1:E:58:SER:O	2.06	0.55
1:A:100:VAL:HG22	1:A:115:ASN:ND2	2.22	0.55
1:B:269:LYS:HA	1:B:273:GLY:O	2.07	0.55
1:C:105:MET:HG3	1:C:105:MET:O	2.06	0.55
1:D:108:GLN:HG3	1:D:160:VAL:CG1	2.36	0.55
1:D:159:ASN:HD21	1:D:161:TYR:HB3	1.70	0.55
1:E:216:GLU:HG3	1:E:276:LYS:HB3	1.88	0.55
1:A:103:THR:HG23	1:A:104:THR:H	1.72	0.55
1:E:7:GLU:HG3	1:E:36:LYS:HD2	1.87	0.55
1:A:212:MET:HG3	1:A:272:LEU:HD21	1.89	0.55
1:C:258:ALA:O	1:C:259:ARG:HD2	2.07	0.55
1:C:289:LYS:HD2	1:C:289:LYS:N	2.21	0.55
1:D:103:THR:HB	1:D:200:THR:HG21	1.89	0.55
1:E:192:PRO:O	1:E:193:ARG:HB2	2.07	0.55
1:E:280:ILE:C	1:E:281:LYS:HD2	2.26	0.55
1:C:103:THR:HB	1:C:200:THR:HG21	1.88	0.55
1:C:227:ARG:NH2	1:C:289:LYS:HB2	2.21	0.55
1:E:269:LYS:HA	1:E:273:GLY:O	2.06	0.55
1:B:44:LYS:O	1:B:45:PHE:HB2	2.05	0.55
1:C:12:THR:HB	1:C:91:PHE:HA	1.89	0.55
1:C:295:ILE:HG23	1:C:299:ILE:HG13	1.89	0.55
1:D:7:GLU:CG	1:D:36:LYS:HD2	2.37	0.55
1:A:103:THR:HG23	1:A:104:THR:N	2.22	0.55
1:A:142:TYR:O	1:A:145:THR:HG23	2.08	0.54
1:B:280:ILE:C	1:B:281:LYS:HD2	2.28	0.54
1:C:226:LEU:HB3	1:C:258:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:HIS:HB2	3:C:385:HOH:O	2.06	0.54
1:D:216:GLU:HG3	1:D:276:LYS:HB3	1.88	0.54
1:D:223:GLY:HA2	1:D:225:GLN:OE1	2.06	0.54
1:D:264:ILE:O	1:D:268:LEU:HB2	2.07	0.54
1:E:7:GLU:CG	1:E:36:LYS:HD2	2.37	0.54
1:D:191:GLY:O	1:D:194:GLU:HG2	2.07	0.54
1:B:223:GLY:HA2	1:B:225:GLN:OE1	2.07	0.54
1:D:288:GLN:CA	1:D:289:LYS:HZ3	2.21	0.54
1:E:105:MET:O	1:E:105:MET:HG3	2.07	0.54
1:B:258:ALA:O	1:B:259:ARG:HD2	2.07	0.54
1:B:263:GLU:O	1:B:267:ILE:HG13	2.08	0.54
1:D:226:LEU:HB3	1:D:258:ALA:HB1	1.88	0.54
1:D:269:LYS:HG2	1:D:275:PHE:CE1	2.42	0.54
1:E:226:LEU:HB3	1:E:258:ALA:HB1	1.88	0.54
1:E:281:LYS:HD2	1:E:281:LYS:N	2.22	0.54
1:A:258:ALA:O	1:A:259:ARG:HD2	2.07	0.54
1:B:12:THR:HB	1:B:91:PHE:HA	1.90	0.54
1:B:295:ILE:CG2	1:B:299:ILE:HD11	2.37	0.54
1:D:269:LYS:HA	1:D:273:GLY:O	2.08	0.54
1:A:46:ARG:HB2	1:A:60:GLY:O	2.08	0.54
1:B:281:LYS:N	1:B:281:LYS:HD2	2.23	0.54
1:C:125:ILE:HD11	3:C:390:HOH:O	2.06	0.54
1:C:202:SER:O	1:C:206:GLN:HG2	2.08	0.53
1:A:254:GLY:H	1:A:295:ILE:HD11	1.72	0.53
1:C:48:ASN:H	1:E:107:ASN:ND2	2.06	0.53
1:E:223:GLY:HA2	1:E:225:GLN:OE1	2.08	0.53
1:E:22:VAL:CG2	2:E:2403:NAD:H51N	2.38	0.53
1:B:289:LYS:N	1:B:289:LYS:HD2	2.23	0.53
1:E:225:GLN:H	1:E:225:GLN:CD	2.11	0.53
1:A:223:GLY:HA2	1:A:225:GLN:OE1	2.09	0.53
1:B:202:SER:O	1:B:206:GLN:HG2	2.07	0.53
1:C:281:LYS:HD2	1:C:281:LYS:N	2.23	0.53
1:E:151:VAL:HG23	1:E:252:ASN:ND2	2.23	0.53
1:B:254:GLY:H	1:B:295:ILE:HD11	1.73	0.53
1:E:159:ASN:ND2	1:E:162:GLY:H	2.06	0.53
1:D:78:ASN:ND2	1:D:118:ALA:HB2	2.24	0.53
1:C:3:TYR:CD1	1:C:237:GLN:HG3	2.44	0.53
1:D:78:ASN:HD21	1:D:114:THR:HA	1.74	0.53
1:E:295:ILE:CG2	1:E:299:ILE:HD11	2.38	0.53
1:A:225:GLN:CD	1:A:225:GLN:H	2.11	0.53
1:B:264:ILE:O	1:B:268:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:GLY:H	1:D:295:ILE:HD11	1.74	0.53
1:B:46:ARG:HA	1:B:58:SER:O	2.08	0.52
1:A:269:LYS:HA	1:A:273:GLY:O	2.09	0.52
1:A:281:LYS:HD2	1:A:281:LYS:N	2.24	0.52
1:D:105:MET:HG3	1:D:105:MET:O	2.08	0.52
1:E:59:LEU:HD11	1:E:101:SER:CB	2.38	0.52
1:A:159:ASN:ND2	1:A:162:GLY:H	2.06	0.52
1:C:267:ILE:HD12	1:C:310:LEU:HG	1.90	0.52
1:E:159:ASN:HD22	1:E:161:TYR:HB3	1.70	0.52
1:C:192:PRO:O	1:C:193:ARG:HB2	2.10	0.52
1:C:142:TYR:O	1:C:145:THR:HG23	2.10	0.52
1:C:237:GLN:HE22	1:C:305:THR:N	2.04	0.52
1:E:107:ASN:OD1	1:E:110:LEU:HD13	2.09	0.52
1:E:207:LEU:HD12	1:E:264:ILE:HG21	1.92	0.52
1:C:108:GLN:HG3	1:C:160:VAL:CG1	2.39	0.52
1:E:78:ASN:HD21	1:E:114:THR:HA	1.74	0.52
1:B:78:ASN:HD21	1:B:114:THR:HA	1.74	0.52
1:A:226:LEU:HB3	1:A:258:ALA:HB1	1.92	0.52
1:E:267:ILE:HD13	1:E:311:GLU:HG3	1.92	0.52
1:B:137:SER:HA	1:B:165:LYS:HD2	1.92	0.51
1:D:267:ILE:HD13	1:D:311:GLU:HG3	1.92	0.51
1:D:108:GLN:HG3	1:D:160:VAL:HG11	1.91	0.51
1:B:225:GLN:CD	1:B:225:GLN:H	2.13	0.51
1:B:269:LYS:HG2	1:B:275:PHE:CE1	2.46	0.51
1:D:212:MET:HG3	1:D:272:LEU:HD21	1.91	0.51
1:E:295:ILE:HG23	1:E:299:ILE:HG13	1.91	0.51
1:B:100:VAL:HG22	1:B:115:ASN:ND2	2.24	0.51
1:A:237:GLN:HE22	1:A:305:THR:N	2.04	0.51
1:C:225:GLN:CD	1:C:225:GLN:H	2.13	0.51
1:D:7:GLU:HG3	1:D:36:LYS:HD2	1.91	0.51
1:E:12:THR:HB	1:E:91:PHE:HA	1.92	0.51
1:B:153:LYS:HE2	1:B:153:LYS:HA	1.91	0.51
1:D:142:TYR:O	1:D:145:THR:HG23	2.10	0.51
1:D:69:LYS:O	1:D:69:LYS:HG3	2.11	0.51
1:A:12:THR:HB	1:A:91:PHE:HA	1.93	0.51
1:B:78:ASN:ND2	1:B:118:ALA:HB2	2.25	0.51
1:E:269:LYS:HG2	1:E:275:PHE:CE1	2.45	0.51
1:D:109:GLU:O	1:D:113:LYS:HG2	2.10	0.51
1:D:42:LEU:HD23	1:D:42:LEU:C	2.30	0.51
1:A:179:ASN:ND2	1:A:180:VAL:H	2.09	0.51
1:C:319:PRO:O	1:C:322:HIS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:MET:HG3	1:C:272:LEU:HD21	1.91	0.50
1:D:151:VAL:HG23	1:D:252:ASN:ND2	2.26	0.50
1:D:295:ILE:CG2	1:D:299:ILE:HD11	2.40	0.50
1:A:295:ILE:HG23	1:A:299:ILE:HG13	1.93	0.50
1:B:237:GLN:HE22	1:B:305:THR:N	2.01	0.50
1:C:9:GLU:HG3	1:C:36:LYS:HD3	1.93	0.50
1:B:7:GLU:HG3	1:B:36:LYS:HD2	1.93	0.50
1:D:286:PHE:N	1:D:286:PHE:CD2	2.78	0.50
1:C:56:PRO:HA	1:C:104:THR:OG1	2.11	0.50
1:D:12:THR:HB	1:D:91:PHE:HA	1.94	0.50
1:E:42:LEU:C	1:E:42:LEU:HD23	2.32	0.50
1:D:267:ILE:HD12	1:D:310:LEU:HG	1.94	0.50
1:D:151:VAL:HG11	1:D:250:VAL:HG22	1.93	0.49
1:B:192:PRO:O	1:B:193:ARG:HB2	2.12	0.49
1:B:218:LYS:C	1:B:218:LYS:HD2	2.32	0.49
1:C:134:ILE:HD12	1:C:134:ILE:N	2.28	0.49
1:E:307:LEU:HB2	1:E:308:TYR:CD2	2.47	0.49
1:B:142:TYR:O	1:B:145:THR:HG23	2.12	0.49
1:A:56:PRO:HA	1:A:104:THR:OG1	2.13	0.49
1:D:208:ALA:O	1:D:212:MET:HG3	2.12	0.49
1:E:267:ILE:HD12	1:E:310:LEU:HG	1.94	0.49
1:B:165:LYS:NZ	2:B:2401:NAD:O3D	2.43	0.49
1:A:78:ASN:HD21	1:A:114:THR:HA	1.76	0.49
1:B:151:VAL:HG11	1:B:250:VAL:HG22	1.94	0.49
1:D:17:GLY:CA	2:D:2401:NAD:H4B	2.42	0.49
1:D:46:ARG:HB2	1:D:60:GLY:O	2.12	0.49
1:B:175:HIS:HE1	1:E:71:GLU:OE2	1.95	0.49
1:B:17:GLY:CA	2:B:2401:NAD:H4B	2.43	0.49
1:C:295:ILE:CG2	1:C:299:ILE:HD11	2.43	0.49
1:E:108:GLN:HG3	1:E:160:VAL:HG11	1.93	0.49
1:E:187:PHE:O	1:E:188:ASN:C	2.51	0.49
1:B:108:GLN:HG3	1:B:160:VAL:CG1	2.43	0.49
1:B:7:GLU:CG	1:B:36:LYS:HD2	2.42	0.49
1:D:295:ILE:HG23	1:D:299:ILE:HG13	1.94	0.49
1:C:255:TYR:HD1	1:C:306:PRO:HB2	1.78	0.49
1:C:46:ARG:HB3	1:E:108:GLN:HB3	1.95	0.49
1:A:242:ALA:HA	1:A:302:LEU:HD22	1.95	0.49
1:C:108:GLN:HG3	1:C:160:VAL:HG11	1.95	0.49
1:C:179:ASN:ND2	1:C:180:VAL:H	2.11	0.49
1:B:208:ALA:O	1:B:212:MET:HG3	2.13	0.48
1:C:203:MET:O	1:C:207:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:GLN:H	1:D:225:GLN:CD	2.15	0.48
1:A:192:PRO:O	1:A:193:ARG:HB2	2.13	0.48
1:B:267:ILE:HD12	1:B:310:LEU:HG	1.95	0.48
1:B:46:ARG:HB3	1:D:108:GLN:HB3	1.93	0.48
1:D:221:GLU:OE2	1:D:282:ASN:N	2.46	0.48
1:D:187:PHE:O	1:D:230:VAL:HG12	2.13	0.48
1:D:287:PHE:C	1:D:289:LYS:NZ	2.66	0.48
1:D:227:ARG:NH2	1:D:289:LYS:HB2	2.28	0.48
1:E:69:LYS:HG3	1:E:69:LYS:O	2.13	0.48
1:A:225:GLN:NE2	1:A:225:GLN:H	2.11	0.48
1:A:269:LYS:HG2	1:A:275:PHE:CE1	2.49	0.48
1:C:133:VAL:C	1:C:134:ILE:HD12	2.33	0.48
1:C:78:ASN:HD21	1:C:114:THR:HA	1.79	0.48
1:E:104:THR:O	1:E:106:LEU:N	2.47	0.48
1:E:134:ILE:N	1:E:134:ILE:HD12	2.29	0.48
1:B:63:LYS:O	1:B:66:ILE:HG12	2.13	0.48
1:C:159:ASN:HD22	1:C:161:TYR:HB3	1.75	0.48
1:E:263:GLU:O	1:E:267:ILE:HG13	2.14	0.48
1:B:207:LEU:HD12	1:B:264:ILE:HG21	1.96	0.48
1:A:124:GLU:OE1	1:D:88:LYS:HE2	2.13	0.48
1:B:255:TYR:HD1	1:B:306:PRO:HB2	1.79	0.47
1:C:207:LEU:HD12	1:C:264:ILE:HG21	1.97	0.47
1:D:237:GLN:HE22	1:D:305:THR:N	2.04	0.47
1:D:230:VAL:HB	1:D:254:GLY:HA2	1.96	0.47
1:A:203:MET:HG3	1:A:261:TYR:CE1	2.49	0.47
1:A:319:PRO:O	1:A:322:HIS:HB2	2.14	0.47
1:C:214:PHE:C	1:C:216:GLU:H	2.17	0.47
1:E:63:LYS:O	1:E:66:ILE:HG12	2.14	0.47
1:D:173:LEU:HD21	1:D:250:VAL:HG13	1.97	0.47
1:A:187:PHE:O	1:A:188:ASN:C	2.52	0.47
1:C:159:ASN:HD21	1:C:161:TYR:HB3	1.74	0.47
1:A:71:GLU:OE2	1:C:175:HIS:HE1	1.98	0.47
1:D:104:THR:O	1:D:106:LEU:N	2.47	0.47
1:C:155:GLU:HG2	1:C:155:GLU:H	1.44	0.47
1:D:203:MET:HG3	1:D:261:TYR:CE1	2.49	0.47
1:A:175:HIS:HE1	1:D:71:GLU:OE2	1.97	0.47
1:E:212:MET:HG3	1:E:272:LEU:HD21	1.96	0.47
1:E:230:VAL:HB	1:E:254:GLY:HA2	1.96	0.47
1:A:108:GLN:HG3	1:A:160:VAL:CG1	2.44	0.47
1:C:269:LYS:HG2	1:C:275:PHE:CE1	2.49	0.47
1:E:294:HIS:NE2	1:E:296:GLU:HG3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:O	1:A:115:ASN:HB2	2.15	0.47
1:C:295:ILE:HG23	1:C:295:ILE:O	2.13	0.47
1:D:296:GLU:HB2	1:D:297:PRO:CD	2.41	0.47
1:E:214:PHE:C	1:E:216:GLU:H	2.16	0.47
1:E:165:LYS:NZ	2:E:2403:NAD:O3D	2.46	0.47
1:A:3:TYR:CD1	1:A:237:GLN:HG3	2.50	0.47
1:B:143:GLY:HA3	1:B:156:SER:O	2.15	0.47
1:C:107:ASN:O	1:C:111:VAL:HG23	2.15	0.47
1:B:227:ARG:HB2	1:B:229:PHE:CZ	2.50	0.47
1:C:209:LEU:CD1	1:C:321:ILE:HG23	2.45	0.47
1:D:295:ILE:HG23	1:D:295:ILE:O	2.15	0.47
1:E:3:TYR:CD1	1:E:237:GLN:HG3	2.50	0.47
1:E:72:VAL:HG12	1:E:73:ILE:N	2.30	0.47
1:B:147:ALA:HB2	1:B:290:HIS:O	2.15	0.46
1:B:203:MET:O	1:B:207:LEU:HG	2.16	0.46
1:A:69:LYS:HD2	1:C:170:GLU:OE1	2.15	0.46
1:B:69:LYS:HG3	1:B:69:LYS:O	2.15	0.46
1:E:100:VAL:N	1:E:115:ASN:HD21	2.04	0.46
1:B:46:ARG:HB2	1:B:60:GLY:O	2.15	0.46
1:D:214:PHE:C	1:D:216:GLU:H	2.18	0.46
1:E:295:ILE:HG23	1:E:295:ILE:O	2.15	0.46
1:B:226:LEU:HB3	1:B:258:ALA:HB1	1.95	0.46
1:C:109:GLU:HG3	1:C:113:LYS:HE2	1.97	0.46
1:D:263:GLU:O	1:D:267:ILE:HG13	2.15	0.46
1:A:295:ILE:CG2	1:A:299:ILE:HD11	2.46	0.46
1:B:203:MET:HG3	1:B:261:TYR:CE1	2.50	0.46
1:C:187:PHE:O	1:C:188:ASN:C	2.54	0.46
1:E:254:GLY:H	1:E:295:ILE:HD11	1.79	0.46
1:B:159:ASN:HD22	1:B:161:TYR:HB3	1.80	0.46
1:B:187:PHE:O	1:B:188:ASN:C	2.54	0.46
1:C:107:ASN:OD1	1:C:110:LEU:HD13	2.15	0.46
1:A:165:LYS:NZ	2:A:2402:NAD:O3D	2.45	0.46
1:C:237:GLN:NE2	1:C:241:LYS:HZ1	2.14	0.46
1:A:267:ILE:HD12	1:A:310:LEU:HG	1.98	0.46
1:B:111:VAL:O	1:B:115:ASN:HB2	2.16	0.46
1:B:134:ILE:N	1:B:134:ILE:HD12	2.31	0.46
1:D:296:GLU:CB	1:D:297:PRO:HD3	2.41	0.46
1:C:69:LYS:O	1:C:69:LYS:HG3	2.16	0.45
1:E:59:LEU:HG	1:E:101:SER:HB3	1.98	0.45
1:A:101:SER:OG	1:A:103:THR:HG22	2.15	0.45
1:B:202:SER:OG	1:B:204:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:GLN:H	1:E:225:GLN:NE2	2.14	0.45
2:E:2403:NAD:O3D	3:E:384:HOH:O	2.07	0.45
1:A:137:SER:O	2:A:2402:NAD:H6N	2.16	0.45
1:A:225:GLN:NE2	1:A:225:GLN:N	2.64	0.45
1:B:230:VAL:HB	1:B:254:GLY:HA2	1.98	0.45
1:A:214:PHE:C	1:A:216:GLU:H	2.20	0.45
1:D:143:GLY:HA3	1:D:156:SER:O	2.17	0.45
1:B:42:LEU:C	1:B:42:LEU:HD23	2.36	0.45
1:C:230:VAL:HB	1:C:254:GLY:HA2	1.98	0.45
1:C:296:GLU:HB2	1:C:297:PRO:CD	2.43	0.45
1:E:143:GLY:HA3	1:E:156:SER:O	2.17	0.45
1:A:72:VAL:HG12	1:A:73:ILE:N	2.31	0.45
1:C:218:LYS:C	1:C:218:LYS:HD2	2.37	0.45
1:C:215:LYS:O	1:C:275:PHE:HB2	2.16	0.45
1:E:319:PRO:O	1:E:322:HIS:HB2	2.16	0.45
1:B:16:THR:OG1	1:B:96:HIS:HA	2.17	0.45
1:B:48:ASN:H	1:D:107:ASN:HD22	1.61	0.45
1:D:294:HIS:NE2	1:D:296:GLU:HG3	2.31	0.45
1:E:242:ALA:HA	1:E:302:LEU:HD22	1.99	0.45
1:B:108:GLN:HG3	1:B:160:VAL:HG11	1.97	0.45
1:B:267:ILE:HD13	1:B:311:GLU:HG3	1.99	0.45
1:E:265:VAL:HG13	1:E:275:PHE:CE2	2.52	0.45
1:E:72:VAL:CG1	1:E:73:ILE:N	2.79	0.45
1:A:104:THR:O	1:A:106:LEU:N	2.50	0.45
1:A:137:SER:HA	1:A:165:LYS:HD2	1.99	0.45
1:B:218:LYS:HD2	1:B:219:LEU:N	2.32	0.45
1:B:307:LEU:HB2	1:B:308:TYR:CD2	2.52	0.45
1:C:95:PHE:HA	1:C:134:ILE:O	2.17	0.45
1:A:230:VAL:HB	1:A:254:GLY:HA2	1.99	0.44
1:B:155:GLU:HG2	1:B:155:GLU:H	1.43	0.44
1:C:83:LEU:HB3	3:C:390:HOH:O	2.16	0.44
1:D:187:PHE:O	1:D:188:ASN:C	2.54	0.44
1:E:133:VAL:C	1:E:134:ILE:HD12	2.38	0.44
1:E:214:PHE:C	1:E:216:GLU:N	2.70	0.44
1:A:116:TYR:O	1:A:119:PHE:HB3	2.17	0.44
1:B:295:ILE:HG23	1:B:299:ILE:HG13	1.98	0.44
1:A:59:LEU:HG	1:A:101:SER:HB3	1.99	0.44
1:B:151:VAL:HG23	1:B:252:ASN:ND2	2.33	0.44
1:B:214:PHE:C	1:B:216:GLU:H	2.19	0.44
1:D:100:VAL:HG22	1:D:115:ASN:ND2	2.32	0.44
1:E:100:VAL:HG22	1:E:115:ASN:ND2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HG23	1:A:252:ASN:ND2	2.32	0.44
1:A:307:LEU:HB2	1:A:308:TYR:CD2	2.52	0.44
1:A:42:LEU:HD23	1:A:42:LEU:C	2.37	0.44
1:B:104:THR:O	1:B:106:LEU:N	2.50	0.44
1:C:214:PHE:C	1:C:216:GLU:N	2.71	0.44
1:C:42:LEU:HD23	1:C:42:LEU:C	2.38	0.44
1:D:3:TYR:CD1	1:D:237:GLN:HG3	2.53	0.44
1:D:302:LEU:O	1:D:303:ASP:HB3	2.17	0.44
1:E:113:LYS:O	1:E:117:GLN:HB3	2.18	0.44
1:D:319:PRO:O	1:D:322:HIS:HB2	2.18	0.44
1:C:143:GLY:HA3	1:C:156:SER:O	2.18	0.44
1:C:63:LYS:O	1:C:66:ILE:HG12	2.17	0.44
1:E:265:VAL:O	1:E:269:LYS:HG3	2.18	0.44
1:A:218:LYS:HD2	1:A:218:LYS:C	2.38	0.44
1:A:237:GLN:HE21	1:A:241:LYS:NZ	2.16	0.44
1:A:69:LYS:O	1:A:69:LYS:HG3	2.18	0.44
1:B:294:HIS:NE2	1:B:296:GLU:HG3	2.31	0.44
1:C:111:VAL:O	1:C:115:ASN:HB2	2.18	0.44
1:D:286:PHE:O	1:D:288:GLN:N	2.49	0.44
1:B:261:TYR:O	1:B:265:VAL:HG23	2.18	0.43
1:B:215:LYS:O	1:B:275:PHE:HB2	2.18	0.43
1:B:319:PRO:O	1:B:322:HIS:HB2	2.18	0.43
1:E:123:LEU:HA	1:E:123:LEU:HD12	1.86	0.43
1:E:314:ILE:O	1:E:318:LEU:HB2	2.18	0.43
1:A:255:TYR:HD1	1:A:306:PRO:HB2	1.83	0.43
1:D:207:LEU:HD12	1:D:264:ILE:HG21	2.01	0.43
1:E:237:GLN:HE22	1:E:305:THR:N	2.03	0.43
1:E:209:LEU:CD1	1:E:321:ILE:HG23	2.48	0.43
1:C:237:GLN:HE21	1:C:241:LYS:NZ	2.16	0.43
1:D:56:PRO:HA	1:D:104:THR:OG1	2.18	0.43
1:E:225:GLN:N	1:E:225:GLN:NE2	2.67	0.43
1:E:56:PRO:HA	1:E:104:THR:OG1	2.18	0.43
1:B:56:PRO:HA	1:B:104:THR:OG1	2.17	0.43
1:C:150:VAL:HG22	1:C:294:HIS:CB	2.48	0.43
1:D:203:MET:O	1:D:207:LEU:HG	2.18	0.43
1:E:179:ASN:ND2	1:E:180:VAL:N	2.65	0.43
1:E:111:VAL:O	1:E:115:ASN:HB2	2.18	0.43
1:B:314:ILE:O	1:B:318:LEU:HB2	2.18	0.43
1:C:104:THR:O	1:C:106:LEU:N	2.51	0.43
1:C:100:VAL:HG22	1:C:115:ASN:ND2	2.34	0.43
1:E:268:LEU:HD12	1:E:268:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:GLU:HA	1:E:36:LYS:HB3	2.00	0.43
1:A:295:ILE:HG23	1:A:295:ILE:O	2.19	0.43
1:B:242:ALA:HA	1:B:302:LEU:HD22	2.01	0.43
1:D:137:SER:HA	1:D:165:LYS:HD2	2.01	0.43
1:D:215:LYS:O	1:D:275:PHE:HB2	2.18	0.43
1:E:302:LEU:O	1:E:303:ASP:HB3	2.19	0.43
1:A:63:LYS:O	1:A:66:ILE:HG12	2.18	0.43
1:C:208:ALA:O	1:C:212:MET:HG3	2.19	0.43
1:C:237:GLN:NE2	1:C:241:LYS:NZ	2.66	0.43
1:E:211:ALA:O	1:E:215:LYS:HA	2.19	0.43
1:B:90:HIS:HB2	3:B:417:HOH:O	2.17	0.43
1:E:227:ARG:HB2	1:E:229:PHE:CZ	2.54	0.43
1:E:310:LEU:O	1:E:314:ILE:HG13	2.19	0.43
1:A:227:ARG:HB2	1:A:229:PHE:CZ	2.54	0.43
1:E:255:TYR:HD1	1:E:306:PRO:HB2	1.83	0.43
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.86	0.42
1:C:225:GLN:NE2	1:C:225:GLN:H	2.17	0.42
1:D:286:PHE:C	1:D:288:GLN:N	2.73	0.42
1:A:151:VAL:HG11	1:A:250:VAL:HG22	2.01	0.42
1:A:72:VAL:CG1	1:A:73:ILE:N	2.81	0.42
1:B:225:GLN:NE2	1:B:225:GLN:H	2.17	0.42
1:E:296:GLU:HB2	1:E:297:PRO:CD	2.37	0.42
1:B:216:GLU:OE1	1:B:276:LYS:HD3	2.18	0.42
1:D:111:VAL:O	1:D:115:ASN:HB2	2.19	0.42
1:D:209:LEU:CD1	1:D:321:ILE:HG23	2.49	0.42
1:D:214:PHE:C	1:D:216:GLU:N	2.73	0.42
1:E:142:TYR:O	1:E:145:THR:HG23	2.19	0.42
1:D:100:VAL:N	1:D:115:ASN:HD21	2.04	0.42
2:D:2401:NAD:H52A	3:D:379:HOH:O	2.19	0.42
1:A:237:GLN:NE2	1:A:241:LYS:NZ	2.67	0.42
1:B:214:PHE:C	1:B:216:GLU:N	2.72	0.42
1:C:270:GLU:HG2	1:C:270:GLU:O	2.20	0.42
1:D:107:ASN:O	1:D:111:VAL:HG23	2.20	0.42
1:D:147:ALA:HB2	1:D:290:HIS:O	2.19	0.42
1:E:147:ALA:HB2	1:E:290:HIS:O	2.18	0.42
1:E:227:ARG:NH2	1:E:289:LYS:HB2	2.34	0.42
1:B:296:GLU:CB	1:B:297:PRO:HD3	2.47	0.42
1:C:173:LEU:HD21	1:C:250:VAL:HG13	2.01	0.42
1:C:261:TYR:O	1:C:265:VAL:HG23	2.19	0.42
1:B:48:ASN:N	1:D:107:ASN:ND2	2.65	0.42
1:D:227:ARG:HB2	1:D:229:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ILE:O	1:D:299:ILE:HG13	2.20	0.42
1:A:216:GLU:OE1	1:A:276:LYS:HD3	2.19	0.42
1:B:9:GLU:HA	1:B:36:LYS:HB3	2.02	0.42
1:C:246:GLN:HE21	1:C:246:GLN:HB2	1.66	0.42
1:D:16:THR:OG1	1:D:96:HIS:HA	2.19	0.42
1:A:9:GLU:HA	1:A:36:LYS:HB3	2.01	0.42
1:A:134:ILE:HD12	1:A:134:ILE:N	2.34	0.42
1:D:12:THR:HA	1:D:38:LYS:HB2	2.02	0.42
1:A:127:ARG:HD3	3:A:371:HOH:O	2.18	0.41
1:A:302:LEU:O	1:A:303:ASP:HB3	2.20	0.41
1:B:133:VAL:C	1:B:134:ILE:HD12	2.41	0.41
1:C:211:ALA:O	1:C:215:LYS:HA	2.20	0.41
1:E:107:ASN:O	1:E:111:VAL:HG23	2.20	0.41
1:A:214:PHE:C	1:A:216:GLU:N	2.74	0.41
1:A:314:ILE:O	1:A:318:LEU:HB2	2.19	0.41
1:D:265:VAL:HG13	1:D:275:PHE:CE2	2.55	0.41
1:C:272:LEU:HD13	1:C:318:LEU:HD21	2.01	0.41
1:A:215:LYS:O	1:A:275:PHE:HB2	2.20	0.41
1:A:268:LEU:HA	1:A:268:LEU:HD12	1.86	0.41
1:B:95:PHE:HA	1:B:134:ILE:O	2.21	0.41
1:B:211:ALA:O	1:B:215:LYS:HA	2.20	0.41
1:E:216:GLU:OE1	1:E:276:LYS:HD3	2.20	0.41
1:D:150:VAL:HG22	1:D:294:HIS:CB	2.51	0.41
1:D:63:LYS:O	1:D:66:ILE:HG12	2.20	0.41
1:A:143:GLY:HA3	1:A:156:SER:O	2.20	0.41
1:B:209:LEU:CD1	1:B:321:ILE:HG23	2.50	0.41
1:C:12:THR:HA	1:C:38:LYS:HB2	2.02	0.41
1:A:108:GLN:HG3	1:A:160:VAL:HG11	2.01	0.41
1:A:296:GLU:HB2	1:A:297:PRO:CD	2.46	0.41
1:C:265:VAL:HG13	1:C:275:PHE:CE2	2.56	0.41
1:C:294:HIS:NE2	1:C:296:GLU:HG3	2.35	0.41
1:D:186:TYR:HD1	1:D:253:VAL:CG1	2.33	0.41
1:A:155:GLU:H	1:A:155:GLU:HG2	1.47	0.41
1:A:16:THR:OG1	1:A:96:HIS:HA	2.20	0.41
1:A:265:VAL:O	1:A:269:LYS:HG3	2.20	0.41
1:A:209:LEU:CD1	1:A:321:ILE:HG23	2.51	0.41
1:D:225:GLN:H	1:D:225:GLN:NE2	2.19	0.41
1:D:268:LEU:HA	1:D:268:LEU:HD12	1.89	0.41
1:A:237:GLN:NE2	1:A:241:LYS:HZ1	2.19	0.41
1:B:302:LEU:O	1:B:303:ASP:HB3	2.21	0.41
1:C:302:LEU:O	1:C:303:ASP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:SER:OG	1:D:103:THR:HG22	2.20	0.41
1:D:294:HIS:NE2	1:D:296:GLU:CG	2.84	0.41
1:D:315:LYS:O	1:D:319:PRO:HD3	2.21	0.41
1:D:7:GLU:HG2	1:D:36:LYS:HD2	2.02	0.41
1:A:146:LYS:HE2	3:A:374:HOH:O	2.19	0.41
1:A:203:MET:O	1:A:207:LEU:HG	2.21	0.41
1:A:7:GLU:HG2	1:A:36:LYS:HD2	2.02	0.41
1:D:242:ALA:HA	1:D:302:LEU:HD22	2.02	0.41
1:B:99:ALA:O	2:B:2401:NAD:H8A	2.21	0.41
1:C:137:SER:HA	1:C:165:LYS:HD2	2.03	0.41
1:C:16:THR:OG1	1:C:96:HIS:HA	2.21	0.41
1:A:78:ASN:OD1	1:A:114:THR:HB	2.21	0.40
1:B:107:ASN:O	1:B:111:VAL:HG23	2.20	0.40
1:C:116:TYR:O	1:C:119:PHE:HB3	2.21	0.40
1:C:59:LEU:HD12	2:C:2403:NAD:O1A	2.21	0.40
1:C:317:TYR:CD2	1:C:321:ILE:HD11	2.57	0.40
1:C:31:GLN:NE2	1:C:69:LYS:N	2.44	0.40
1:E:294:HIS:NE2	1:E:296:GLU:CG	2.84	0.40
1:A:100:VAL:HG22	1:A:115:ASN:HD21	1.86	0.40
1:B:107:ASN:OD1	1:B:110:LEU:HD13	2.21	0.40
1:D:101:SER:CB	1:D:103:THR:HG22	2.52	0.40
1:D:109:GLU:HG2	1:D:110:LEU:HD12	2.02	0.40
1:E:207:LEU:HD12	1:E:264:ILE:CG2	2.51	0.40
1:E:218:LYS:C	1:E:218:LYS:HD2	2.42	0.40
1:A:186:TYR:HD1	1:A:253:VAL:CG1	2.34	0.40
1:A:261:TYR:O	1:A:265:VAL:HG23	2.21	0.40
1:B:89:LEU:O	1:B:129:LYS:HE3	2.21	0.40
1:C:314:ILE:O	1:C:318:LEU:HB2	2.21	0.40
1:A:219:LEU:O	1:A:279:TYR:HA	2.21	0.40
1:D:42:LEU:HD23	1:D:43:ASP:N	2.36	0.40
1:B:113:LYS:O	1:B:117:GLN:HB3	2.22	0.40
1:E:155:GLU:HG2	1:E:155:GLU:H	1.45	0.40
1:E:219:LEU:O	1:E:279:TYR:HA	2.21	0.40
1:E:95:PHE:HA	1:E:134:ILE: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	304/362 (84%)	267 (88%)	31 (10%)	6 (2%)	7	8
1	B	305/362 (84%)	269 (88%)	29 (10%)	7 (2%)	6	6
1	C	304/362 (84%)	268 (88%)	29 (10%)	7 (2%)	6	6
1	D	308/362 (85%)	271 (88%)	29 (9%)	8 (3%)	5	5
1	E	304/362 (84%)	267 (88%)	30 (10%)	7 (2%)	6	6
All	All	1525/1810 (84%)	1342 (88%)	148 (10%)	35 (2%)	6	6

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	PHE
1	A	221	GLU
1	B	45	PHE
1	B	221	GLU
1	C	45	PHE
1	C	221	GLU
1	D	45	PHE
1	D	221	GLU
1	E	45	PHE
1	E	221	GLU
1	A	21	PHE
1	B	21	PHE
1	C	21	PHE
1	D	21	PHE
1	D	46	ARG
1	D	287	PHE
1	E	21	PHE
1	E	308	TYR
1	A	46	ARG
1	A	188	ASN
1	A	308	TYR

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Mol	Chain	Res	Type
1	B	188	ASN
1	B	308	TYR
1	C	46	ARG
1	C	188	ASN
1	C	222	PHE
1	C	308	TYR
1	D	308	TYR
1	E	46	ARG
1	E	188	ASN
1	B	46	ARG
1	B	222	PHE
1	D	188	ASN
1	D	222	PHE
1	E	222	PHE

### 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	268/313 (86%)	249 (93%)	19 (7%)	14	19
1	B	269/313 (86%)	251 (93%)	18 (7%)	16	21
1	C	268/313 (86%)	250 (93%)	18 (7%)	16	21
1	D	272/313 (87%)	255 (94%)	17 (6%)	18	23
1	E	268/313 (86%)	252 (94%)	16 (6%)	19	25
All	All	1345/1565 (86%)	1257 (94%)	88 (6%)	17	23

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	59	LEU
1	A	81	LEU
1	A	83	LEU
1	A	114	THR

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	155	GLU
1	A	160	VAL
1	A	179	ASN
1	A	184	LEU
1	A	205	LEU
1	A	209	LEU
1	A	218	LYS
1	A	221	GLU
1	A	224	GLU
1	A	225	GLN
1	A	278	THR
1	A	281	LYS
1	A	295	ILE
1	B	40	VAL
1	B	59	LEU
1	B	81	LEU
1	B	83	LEU
1	B	114	THR
1	B	123	LEU
1	B	155	GLU
1	B	156	SER
1	B	160	VAL
1	B	184	LEU
1	B	209	LEU
1	B	218	LYS
1	B	221	GLU
1	B	224	GLU
1	B	225	GLN
1	B	278	THR
1	B	281	LYS
1	B	295	ILE
1	C	40	VAL
1	C	59	LEU
1	C	81	LEU
1	C	83	LEU
1	C	114	THR
1	C	123	LEU
1	C	155	GLU
1	C	160	VAL
1	C	184	LEU
1	C	209	LEU

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Mol	Chain	Res	Type
1	C	218	LYS
1	C	221	GLU
1	C	224	GLU
1	C	225	GLN
1	C	278	THR
1	C	281	LYS
1	C	295	ILE
1	C	309	ASP
1	D	40	VAL
1	D	81	LEU
1	D	83	LEU
1	D	114	THR
1	D	123	LEU
1	D	155	GLU
1	D	184	LEU
1	D	209	LEU
1	D	218	LYS
1	D	221	GLU
1	D	224	GLU
1	D	225	GLN
1	D	240	VAL
1	D	278	THR
1	D	281	LYS
1	D	286	PHE
1	D	295	ILE
1	E	40	VAL
1	E	59	LEU
1	E	81	LEU
1	E	83	LEU
1	E	114	THR
1	E	123	LEU
1	E	155	GLU
1	E	184	LEU
1	E	209	LEU
1	E	218	LYS
1	E	221	GLU
1	E	224	GLU
1	E	225	GLN
1	E	278	THR
1	E	281	LYS
1	E	295	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	31	GLN
1	A	34	HIS
1	A	61	HIS
1	A	78	ASN
1	A	115	ASN
1	A	121	ASN
1	A	159	ASN
1	A	175	HIS
1	A	179	ASN
1	A	181	GLN
1	A	225	GLN
1	A	237	GLN
1	A	239	ASN
1	A	246	GLN
1	A	262	ASN
1	A	271	HIS
1	A	290	HIS
1	B	11	GLN
1	B	31	GLN
1	B	34	HIS
1	B	61	HIS
1	B	115	ASN
1	B	117	GLN
1	B	121	ASN
1	B	159	ASN
1	B	175	HIS
1	B	179	ASN
1	B	225	GLN
1	B	237	GLN
1	B	239	ASN
1	B	246	GLN
1	B	262	ASN
1	B	271	HIS
1	C	31	GLN
1	C	61	HIS
1	C	78	ASN
1	C	115	ASN
1	C	117	GLN
1	C	121	ASN
1	C	159	ASN
1	C	175	HIS

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Mol	Chain	Res	Type
1	C	179	ASN
1	C	225	GLN
1	C	237	GLN
1	C	239	ASN
1	C	246	GLN
1	C	262	ASN
1	C	271	HIS
1	D	31	GLN
1	D	61	HIS
1	D	107	ASN
1	D	115	ASN
1	D	117	GLN
1	D	121	ASN
1	D	159	ASN
1	D	179	ASN
1	D	181	GLN
1	D	225	GLN
1	D	237	GLN
1	D	239	ASN
1	D	246	GLN
1	D	257	GLN
1	D	262	ASN
1	D	271	HIS
1	D	290	HIS
1	E	31	GLN
1	E	34	HIS
1	E	61	HIS
1	E	115	ASN
1	E	121	ASN
1	E	159	ASN
1	E	179	ASN
1	E	225	GLN
1	E	237	GLN
1	E	239	ASN
1	E	246	GLN
1	E	262	ASN
1	E	271	HIS
1	E	290	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 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	2402	-	42,48,48	1.28	4 (9%)	50,73,73	1.47	7 (14%)
2	NAD	B	2401	-	42,48,48	1.44	5 (11%)	50,73,73	1.60	9 (18%)
2	NAD	C	2403	-	42,48,48	1.15	4 (9%)	50,73,73	1.55	8 (16%)
2	NAD	D	2401	-	42,48,48	1.22	5 (11%)	50,73,73	1.69	9 (18%)
2	NAD	E	2403	-	42,48,48	1.14	5 (11%)	50,73,73	1.51	8 (16%)

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	2402	-	-	8/26/62/62	0/5/5/5
2	NAD	B	2401	-	-	9/26/62/62	0/5/5/5
2	NAD	C	2403	-	-	6/26/62/62	0/5/5/5
2	NAD	D	2401	-	-	6/26/62/62	0/5/5/5
2	NAD	E	2403	-	-	7/26/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2401	NAD	O3D-C3D	5.74	1.56	1.43
2	E	2403	NAD	C2N-N1N	4.61	1.40	1.35
2	B	2401	NAD	C2N-N1N	4.57	1.40	1.35
2	C	2403	NAD	C2N-N1N	4.50	1.40	1.35
2	A	2402	NAD	C2N-N1N	4.45	1.40	1.35
2	D	2401	NAD	C2N-N1N	4.43	1.40	1.35
2	A	2402	NAD	O3D-C3D	4.06	1.52	1.43
2	D	2401	NAD	O3D-C3D	-3.10	1.35	1.43
2	E	2403	NAD	O4D-C1D	2.38	1.44	1.41
2	C	2403	NAD	O4D-C1D	2.35	1.44	1.41
2	D	2401	NAD	O4D-C1D	2.30	1.44	1.41
2	A	2402	NAD	O4D-C1D	2.28	1.44	1.41
2	B	2401	NAD	O4D-C1D	2.26	1.44	1.41
2	E	2403	NAD	O4B-C1B	2.19	1.44	1.41
2	A	2402	NAD	C6N-N1N	2.16	1.40	1.35
2	C	2403	NAD	C6N-N1N	2.14	1.40	1.35
2	E	2403	NAD	C3N-C7N	2.11	1.53	1.50
2	D	2401	NAD	C6N-N1N	2.11	1.40	1.35
2	B	2401	NAD	C6N-N1N	2.10	1.40	1.35
2	E	2403	NAD	C6N-N1N	2.09	1.40	1.35
2	B	2401	NAD	O4B-C1B	2.08	1.44	1.41
2	D	2401	NAD	O4B-C1B	2.08	1.44	1.41
2	C	2403	NAD	O4B-C1B	2.06	1.44	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2401	NAD	O4B-C1B-C2B	-5.65	98.67	106.93
2	C	2403	NAD	O3D-C3D-C2D	5.15	128.47	111.82
2	D	2401	NAD	O3D-C3D-C2D	5.00	127.99	111.82
2	B	2401	NAD	O4B-C1B-C2B	-4.56	100.26	106.93
2	E	2403	NAD	O3D-C3D-C2D	4.49	126.36	111.82
2	D	2401	NAD	N3A-C2A-N1A	-4.48	121.67	128.68
2	B	2401	NAD	N3A-C2A-N1A	-4.46	121.71	128.68
2	A	2402	NAD	N3A-C2A-N1A	-4.44	121.74	128.68
2	E	2403	NAD	N3A-C2A-N1A	-4.42	121.77	128.68
2	C	2403	NAD	N3A-C2A-N1A	-4.40	121.80	128.68
2	B	2401	NAD	O3D-C3D-C2D	4.36	125.94	111.82
2	C	2403	NAD	O4B-C1B-C2B	-3.98	101.11	106.93
2	E	2403	NAD	O4B-C1B-C2B	-3.97	101.12	106.93
2	A	2402	NAD	O4B-C1B-C2B	-3.72	101.50	106.93
2	A	2402	NAD	PN-O3-PA	-3.56	120.60	132.83
2	A	2402	NAD	O3D-C3D-C2D	3.32	122.55	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2401	NAD	O3D-C3D-C4D	3.22	120.37	111.05
2	D	2401	NAD	O4D-C1D-C2D	-2.98	102.57	106.93
2	D	2401	NAD	C3D-C2D-C1D	-2.98	96.49	100.98
2	B	2401	NAD	PN-O3-PA	-2.96	122.68	132.83
2	E	2403	NAD	PN-O3-PA	-2.91	122.86	132.83
2	B	2401	NAD	C3D-C2D-C1D	-2.90	96.61	100.98
2	A	2402	NAD	C3D-C2D-C1D	-2.90	96.62	100.98
2	D	2401	NAD	PN-O3-PA	-2.87	122.98	132.83
2	C	2403	NAD	PN-O3-PA	-2.83	123.11	132.83
2	E	2403	NAD	O4D-C1D-C2D	-2.67	103.03	106.93
2	E	2403	NAD	C3N-C7N-N7N	-2.46	114.80	117.75
2	B	2401	NAD	C3N-C7N-N7N	-2.43	114.83	117.75
2	C	2403	NAD	C6N-N1N-C2N	-2.43	119.76	121.97
2	C	2403	NAD	C3D-C2D-C1D	-2.40	97.36	100.98
2	E	2403	NAD	C6N-N1N-C2N	-2.39	119.79	121.97
2	B	2401	NAD	O4D-C1D-C2D	-2.31	103.54	106.93
2	C	2403	NAD	O4D-C1D-C2D	-2.31	103.55	106.93
2	D	2401	NAD	C6N-N1N-C2N	-2.31	119.87	121.97
2	A	2402	NAD	O4D-C1D-C2D	-2.25	103.63	106.93
2	D	2401	NAD	C4A-C5A-N7A	-2.25	107.05	109.40
2	E	2403	NAD	C3D-C2D-C1D	-2.17	97.71	100.98
2	A	2402	NAD	C3N-C7N-N7N	-2.13	115.19	117.75
2	D	2401	NAD	C3N-C7N-N7N	-2.12	115.21	117.75
2	C	2403	NAD	C3N-C7N-N7N	-2.05	115.29	117.75
2	B	2401	NAD	C4A-C5A-N7A	-2.00	107.31	109.40

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2402	NAD	C5B-O5B-PA-O1A
2	A	2402	NAD	C5D-O5D-PN-O2N
2	B	2401	NAD	C5B-O5B-PA-O2A
2	B	2401	NAD	C5D-O5D-PN-O2N
2	C	2403	NAD	C5D-O5D-PN-O1N
2	C	2403	NAD	C5D-O5D-PN-O2N
2	D	2401	NAD	C5D-O5D-PN-O1N
2	D	2401	NAD	C5D-O5D-PN-O2N
2	E	2403	NAD	C5D-O5D-PN-O1N
2	E	2403	NAD	C5D-O5D-PN-O2N
2	B	2401	NAD	O4D-C4D-C5D-O5D
2	B	2401	NAD	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	C	2403	NAD	PN-O3-PA-O5B
2	E	2403	NAD	PN-O3-PA-O5B
2	A	2402	NAD	C5D-O5D-PN-O3
2	B	2401	NAD	C5B-O5B-PA-O3
2	B	2401	NAD	C5D-O5D-PN-O3
2	A	2402	NAD	C5D-O5D-PN-O1N
2	B	2401	NAD	C5B-O5B-PA-O1A
2	B	2401	NAD	C5D-O5D-PN-O1N
2	A	2402	NAD	PA-O3-PN-O2N
2	D	2401	NAD	PA-O3-PN-O2N
2	B	2401	NAD	PA-O3-PN-O2N
2	A	2402	NAD	O4B-C4B-C5B-O5B
2	A	2402	NAD	C5B-O5B-PA-O3
2	C	2403	NAD	C5D-O5D-PN-O3
2	D	2401	NAD	C5B-O5B-PA-O3
2	D	2401	NAD	C5D-O5D-PN-O3
2	E	2403	NAD	C5D-O5D-PN-O3
2	C	2403	NAD	O4B-C4B-C5B-O5B
2	A	2402	NAD	PA-O3-PN-O1N
2	C	2403	NAD	PA-O3-PN-O1N
2	E	2403	NAD	PA-O3-PN-O1N
2	E	2403	NAD	PA-O3-PN-O2N
2	D	2401	NAD	C5B-O5B-PA-O1A
2	E	2403	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

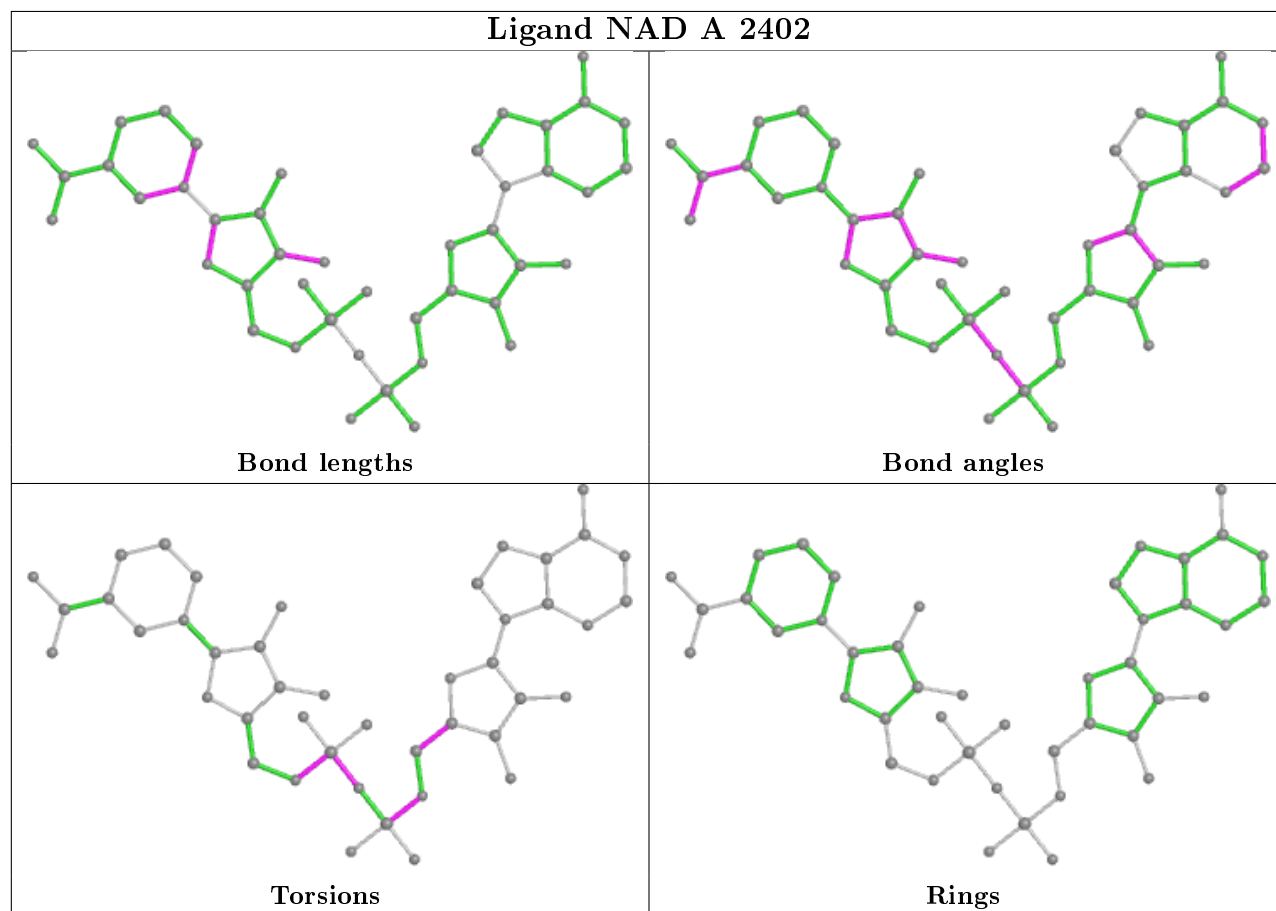
5 monomers are involved in 22 short contacts:

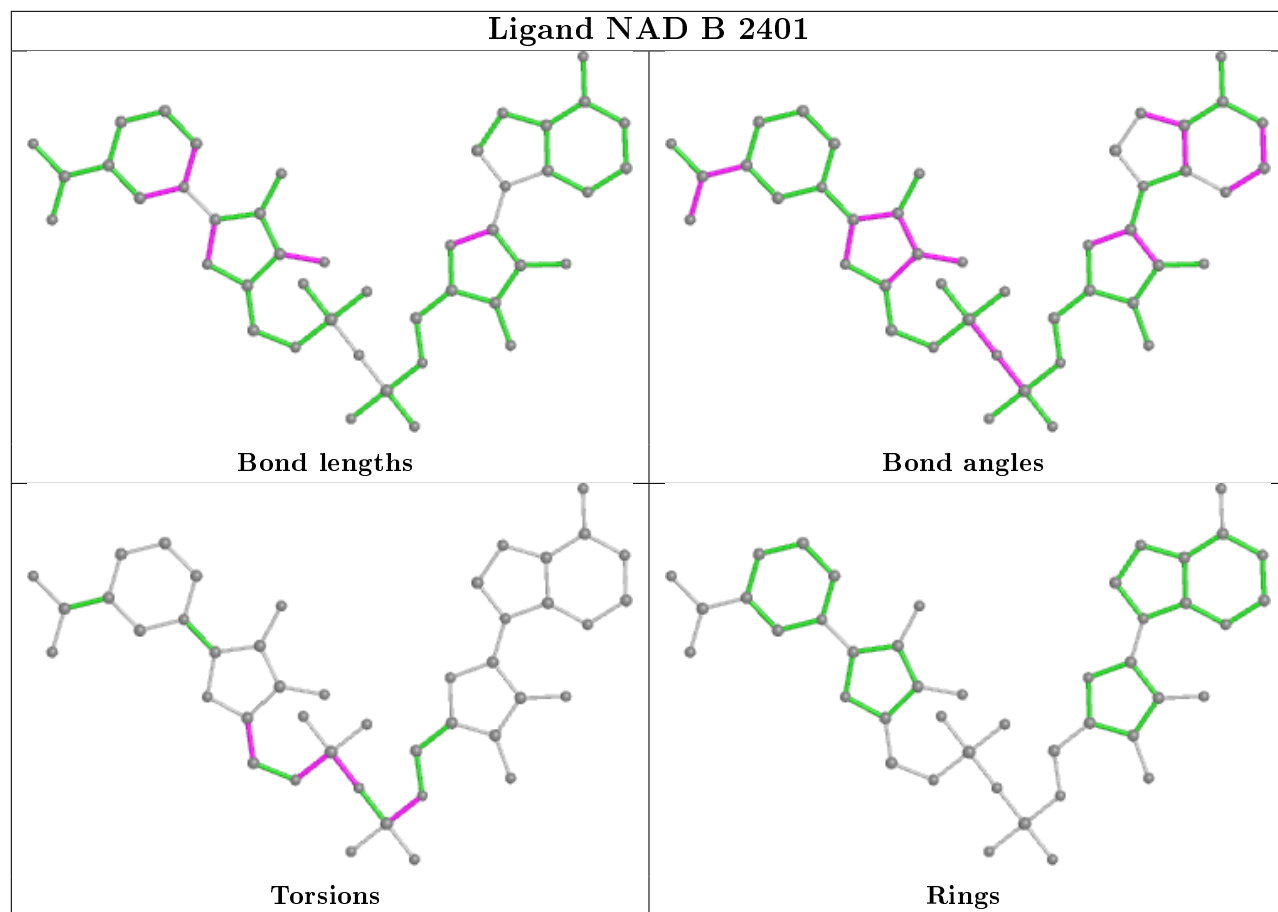
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2402	NAD	3	0
2	B	2401	NAD	6	0
2	C	2403	NAD	4	0
2	D	2401	NAD	4	0
2	E	2403	NAD	5	0

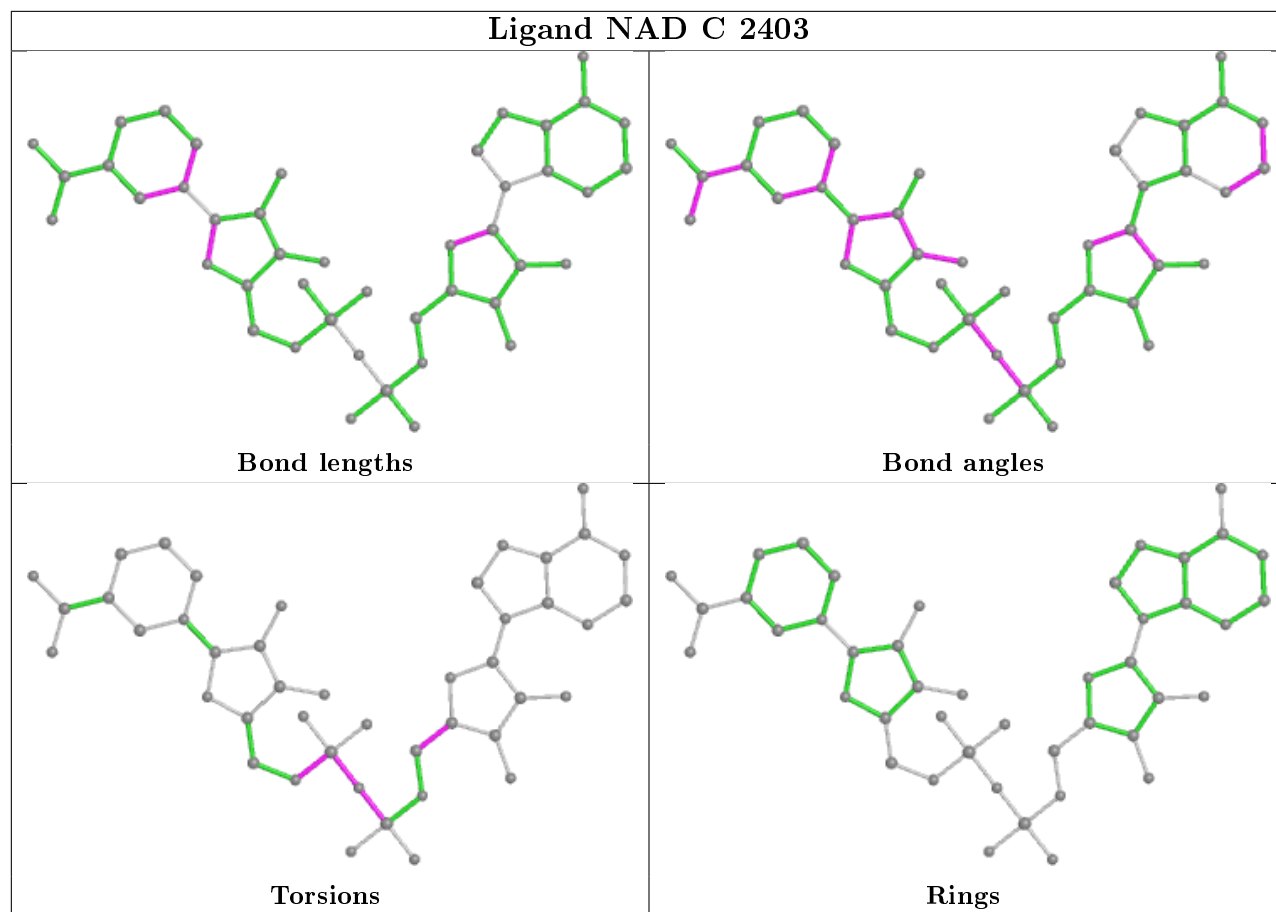
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

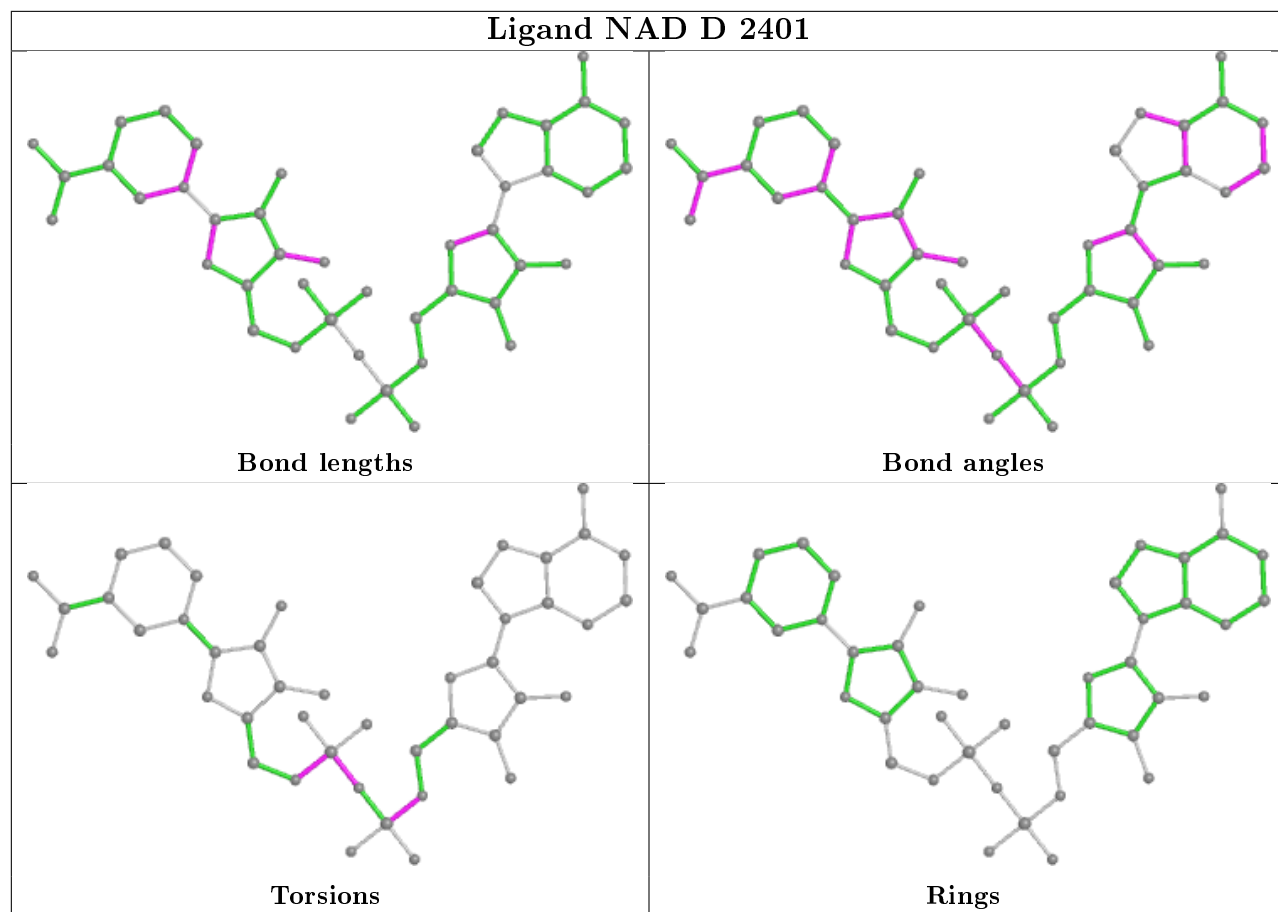


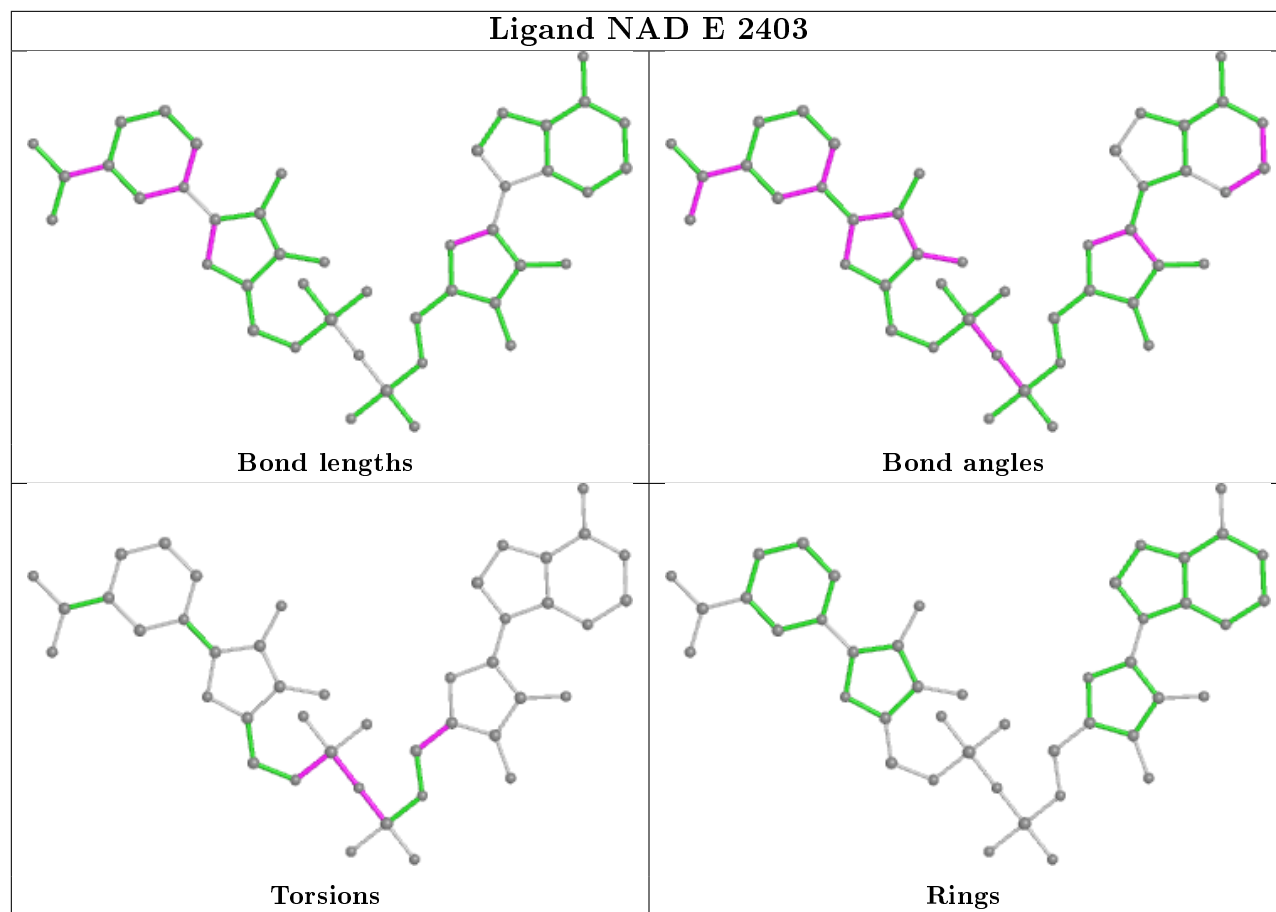
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	310/362 (85%)	0.65	25 (8%) 12 15	27, 46, 86, 100	0
1	B	311/362 (85%)	0.49	15 (4%) 30 37	26, 46, 87, 100	0
1	C	310/362 (85%)	0.71	43 (13%) 2 3	29, 48, 87, 102	0
1	D	314/362 (86%)	0.62	28 (8%) 9 11	27, 47, 88, 101	0
1	E	310/362 (85%)	0.61	31 (10%) 7 9	30, 48, 87, 101	0
All	All	1555/1810 (85%)	0.62	142 (9%) 9 11	26, 47, 88, 102	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	THR	7.8
1	D	222	PHE	7.6
1	A	104	THR	7.4
1	A	56	PRO	6.5
1	E	220	PHE	6.3
1	C	104	THR	6.1
1	C	222	PHE	6.0
1	E	219	LEU	5.9
1	B	56	PRO	5.7
1	E	226	LEU	5.5
1	A	106	LEU	5.2
1	E	222	PHE	5.1
1	C	105	MET	5.1
1	C	264	ILE	5.0
1	D	104	THR	4.8
1	E	223	GLY	4.8
1	C	226	LEU	4.7
1	D	281	LYS	4.7
1	C	56	PRO	4.6
1	C	106	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	214	PHE	4.6
1	A	219	LEU	4.6
1	D	220	PHE	4.6
1	A	214	PHE	4.5
1	A	103	THR	4.5
1	B	105	MET	4.5
1	C	213	ALA	4.4
1	E	275	PHE	4.4
1	D	223	GLY	4.4
1	C	279	TYR	4.3
1	C	272	LEU	4.3
1	C	280	ILE	4.3
1	C	207	LEU	4.2
1	C	322	HIS	4.2
1	D	280	ILE	4.1
1	E	103	THR	4.1
1	C	217	VAL	4.0
1	C	211	ALA	4.0
1	A	222	PHE	3.9
1	E	56	PRO	3.9
1	E	281	LYS	3.8
1	C	219	LEU	3.8
1	C	277	VAL	3.8
1	C	214	PHE	3.7
1	C	221	GLU	3.7
1	D	217	VAL	3.7
1	D	277	VAL	3.7
1	D	278	THR	3.7
1	C	321	ILE	3.7
1	E	215	LYS	3.7
1	E	217	VAL	3.7
1	A	105	MET	3.6
1	B	103	THR	3.6
1	A	280	ILE	3.4
1	C	273	GLY	3.4
1	C	276	LYS	3.4
1	D	275	PHE	3.4
1	A	220	PHE	3.3
1	E	279	TYR	3.3
1	D	282	ASN	3.3
1	D	56	PRO	3.3
1	B	217	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	277	VAL	3.3
1	E	276	LYS	3.2
1	D	218	LYS	3.2
1	D	261	TYR	3.2
1	C	269	LYS	3.2
1	E	4	ILE	3.2
1	D	279	TYR	3.1
1	C	281	LYS	3.1
1	A	223	GLY	3.1
1	C	289	LYS	3.1
1	B	222	PHE	3.0
1	A	226	LEU	3.0
1	E	213	ALA	2.9
1	E	290	HIS	2.9
1	D	214	PHE	2.8
1	C	103	THR	2.8
1	B	214	PHE	2.8
1	E	104	THR	2.8
1	A	247	LYS	2.8
1	D	215	LYS	2.8
1	C	275	PHE	2.7
1	D	324	ILE	2.7
1	D	209	LEU	2.7
1	A	276	LYS	2.7
1	C	59	LEU	2.7
1	C	215	LYS	2.7
1	C	225	GLN	2.7
1	B	219	LEU	2.6
1	E	221	GLU	2.6
1	B	289	LYS	2.6
1	E	264	ILE	2.6
1	A	272	LEU	2.6
1	C	318	LEU	2.6
1	E	209	LEU	2.6
1	D	105	MET	2.6
1	E	102	ASP	2.6
1	A	275	PHE	2.5
1	D	276	LYS	2.5
1	D	288	GLN	2.5
1	E	261	TYR	2.5
1	B	275	PHE	2.5
1	B	57	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	270	GLU	2.5
1	B	278	THR	2.5
1	E	218	LYS	2.5
1	C	324	ILE	2.4
1	E	59	LEU	2.4
1	E	105	MET	2.4
1	D	216	GLU	2.4
1	D	103	THR	2.4
1	A	216	GLU	2.4
1	C	208	ALA	2.4
1	E	322	HIS	2.3
1	A	218	LYS	2.3
1	B	276	LYS	2.3
1	A	277	VAL	2.3
1	C	204	VAL	2.3
1	A	278	THR	2.3
1	A	221	GLU	2.3
1	B	277	VAL	2.3
1	C	1	MET	2.3
1	C	317	TYR	2.3
1	C	206	GLN	2.2
1	A	281	LYS	2.2
1	C	261	TYR	2.2
1	E	101	SER	2.2
1	C	220	PHE	2.2
1	D	287	PHE	2.2
1	D	212	MET	2.1
1	C	218	LYS	2.1
1	C	274	ASP	2.1
1	E	208	ALA	2.1
1	D	318	LEU	2.1
1	A	319	PRO	2.1
1	C	278	THR	2.1
1	A	246	GLN	2.1
1	D	4	ILE	2.0
1	E	148	PRO	2.0
1	B	215	LYS	2.0
1	A	279	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

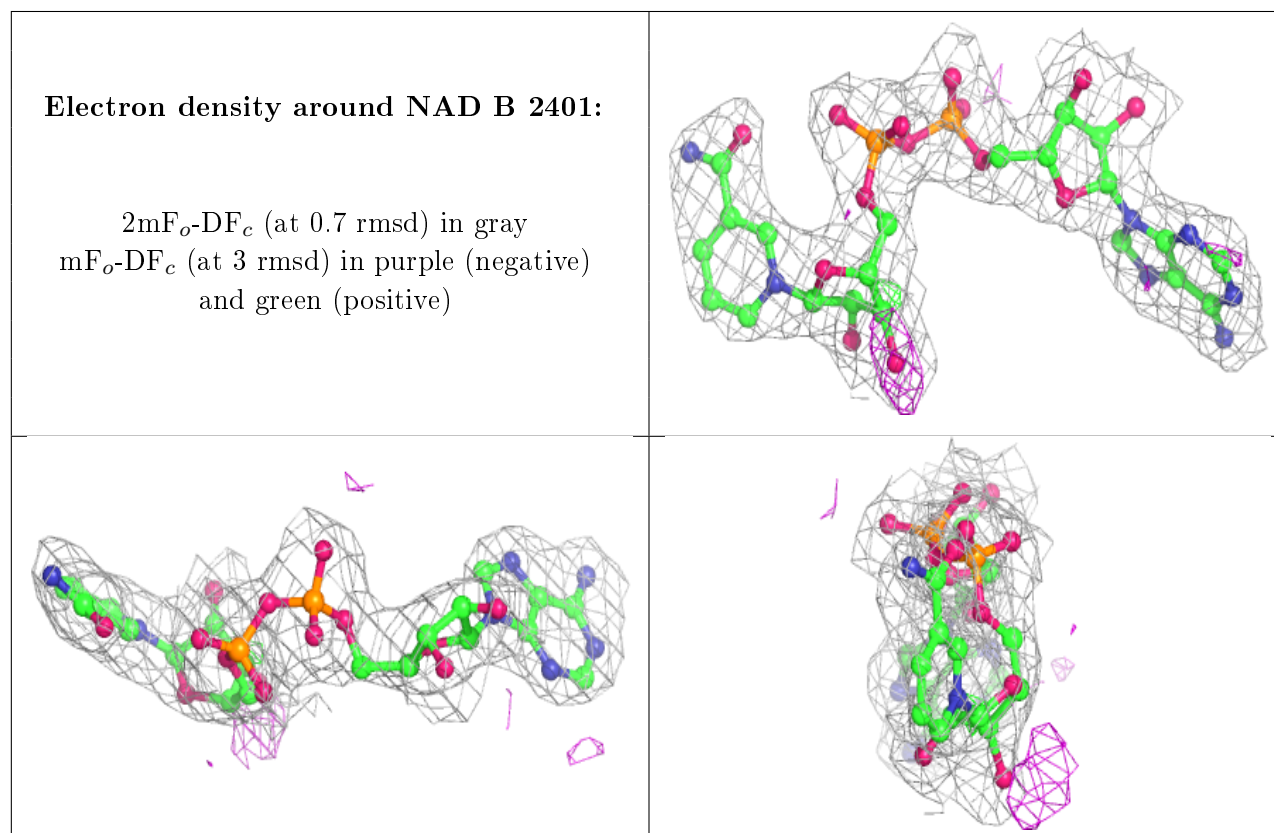
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

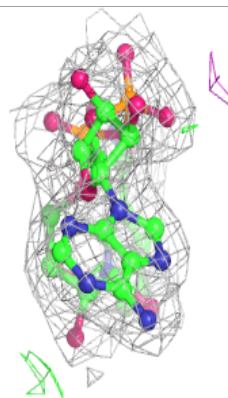
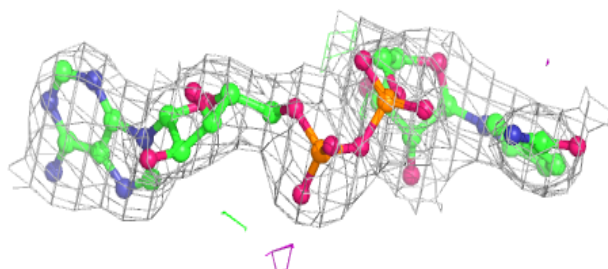
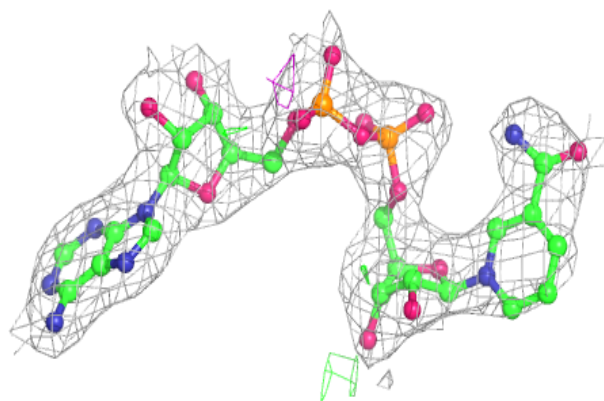
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	B	2401	44/44	0.96	0.17	35,39,51,53	0
2	NAD	C	2403	44/44	0.96	0.18	40,51,62,63	0
2	NAD	D	2401	44/44	0.96	0.17	27,35,45,49	0
2	NAD	E	2403	44/44	0.96	0.14	43,47,57,58	0
2	NAD	A	2402	44/44	0.97	0.15	30,35,44,49	0

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.

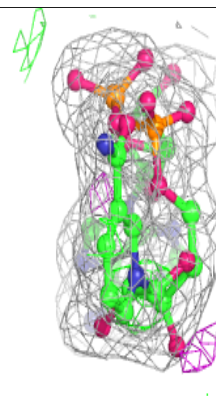
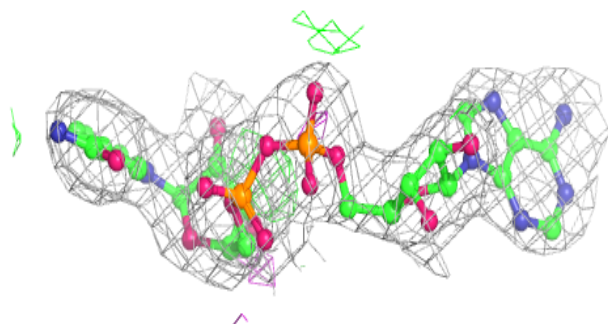
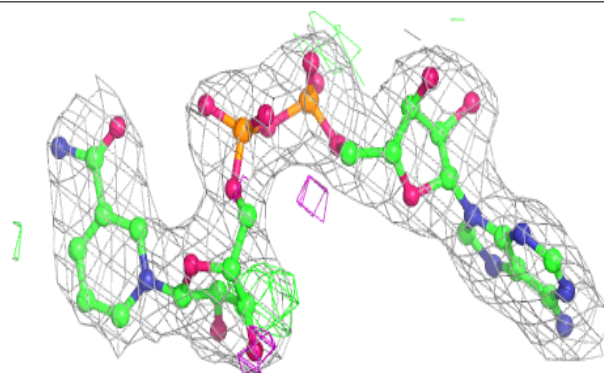


**Electron density around NAD C 2403:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

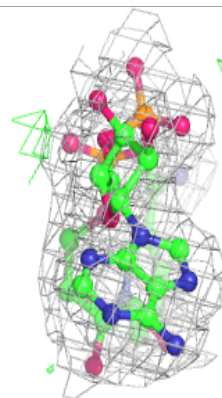
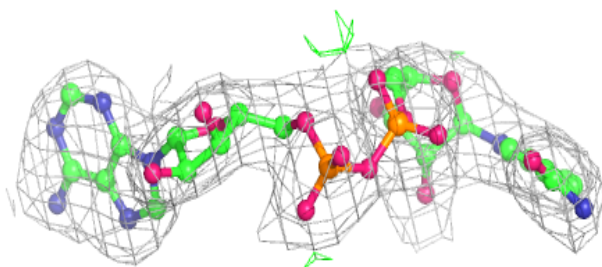
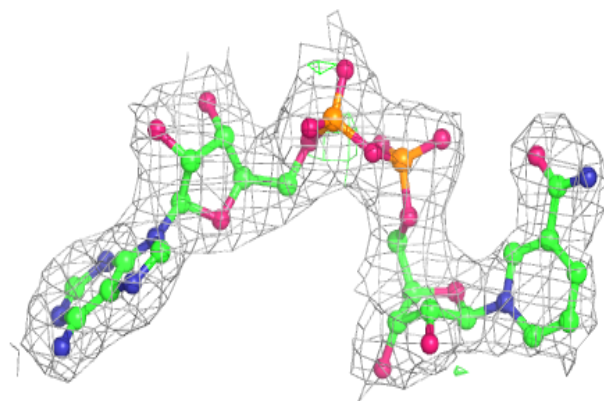
**Electron density around NAD D 2401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

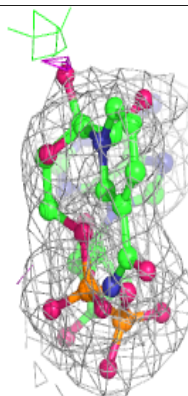
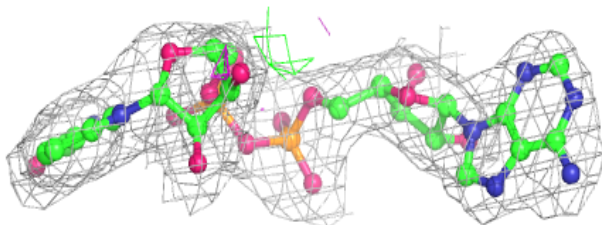
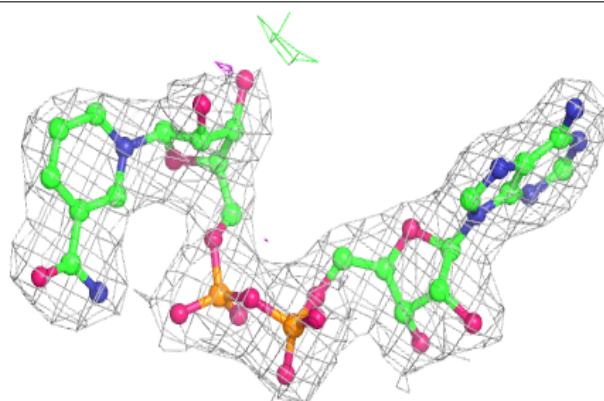


**Electron density around NAD E 2403:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAD A 2402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.