Full wwPDB X-ray Structure Validation Report (i)

Jan 9, 2024 – 03:57 PM EST

PDB ID	:	6PX2
Title	:	Acropora millepora GAPDH
Authors	:	Brandt, G.S.; Fields, P.A.
Deposited on	:	2019-07-24
Resolution	:	2.40 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 (i)) were used in the production of this report:

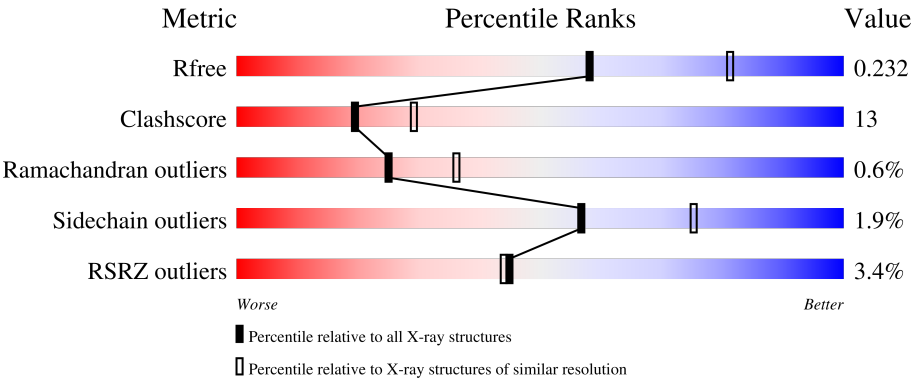
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	355	3% 76% 15% • 6%
1	B	355	5% 64% 27% • 6%
1	C	355	5% 79% 14% • 6%
1	D	355	3% 74% 17% • 6%
1	E	355	2% 74% 18% • 6%

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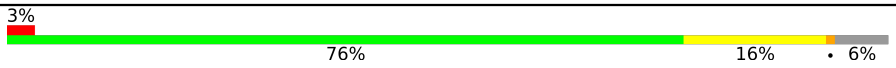
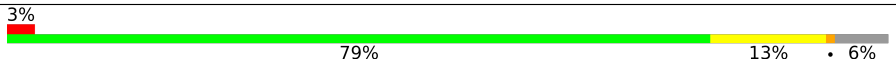
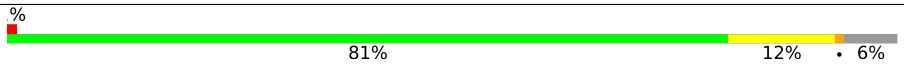
Mol	Chain	Length	Quality of chain
1	F	355	
1	G	355	
1	H	355	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20862 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2531	1610	423	486	12			
1	B	332	Total	C	N	O	S	0	0	0
			2530	1610	422	486	12			
1	C	332	Total	C	N	O	S	0	0	0
			2531	1610	423	486	12			
1	D	332	Total	C	N	O	S	0	0	0
			2531	1610	423	486	12			
1	E	332	Total	C	N	O	S	0	0	0
			2531	1610	423	486	12			
1	F	332	Total	C	N	O	S	0	0	0
			2531	1610	423	486	12			
1	G	332	Total	C	N	O	S	0	0	0
			2531	1610	423	486	12			
1	H	332	Total	C	N	O	S	0	0	0
			2531	1610	423	486	12			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A3F2YLZ0
A	334	ALA	-	expression tag	UNP A0A3F2YLZ0
A	335	GLU	-	expression tag	UNP A0A3F2YLZ0
A	336	ASN	-	expression tag	UNP A0A3F2YLZ0
A	337	LEU	-	expression tag	UNP A0A3F2YLZ0
A	338	TYR	-	expression tag	UNP A0A3F2YLZ0
A	339	PHE	-	expression tag	UNP A0A3F2YLZ0
A	340	GLN	-	expression tag	UNP A0A3F2YLZ0
A	341	SER	-	expression tag	UNP A0A3F2YLZ0
A	342	HIS	-	expression tag	UNP A0A3F2YLZ0
A	343	HIS	-	expression tag	UNP A0A3F2YLZ0
A	344	HIS	-	expression tag	UNP A0A3F2YLZ0
A	345	HIS	-	expression tag	UNP A0A3F2YLZ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	346	HIS	-	expression tag	UNP A0A3F2YLZ0
A	347	HIS	-	expression tag	UNP A0A3F2YLZ0
A	348	ASP	-	expression tag	UNP A0A3F2YLZ0
A	349	TYR	-	expression tag	UNP A0A3F2YLZ0
A	350	LYS	-	expression tag	UNP A0A3F2YLZ0
A	351	ASP	-	expression tag	UNP A0A3F2YLZ0
A	352	ASP	-	expression tag	UNP A0A3F2YLZ0
A	353	ASP	-	expression tag	UNP A0A3F2YLZ0
A	354	ASP	-	expression tag	UNP A0A3F2YLZ0
A	355	LYS	-	expression tag	UNP A0A3F2YLZ0
B	1	MET	-	initiating methionine	UNP A0A3F2YLZ0
B	334	ALA	-	expression tag	UNP A0A3F2YLZ0
B	335	GLU	-	expression tag	UNP A0A3F2YLZ0
B	336	ASN	-	expression tag	UNP A0A3F2YLZ0
B	337	LEU	-	expression tag	UNP A0A3F2YLZ0
B	338	TYR	-	expression tag	UNP A0A3F2YLZ0
B	339	PHE	-	expression tag	UNP A0A3F2YLZ0
B	340	GLN	-	expression tag	UNP A0A3F2YLZ0
B	341	SER	-	expression tag	UNP A0A3F2YLZ0
B	342	HIS	-	expression tag	UNP A0A3F2YLZ0
B	343	HIS	-	expression tag	UNP A0A3F2YLZ0
B	344	HIS	-	expression tag	UNP A0A3F2YLZ0
B	345	HIS	-	expression tag	UNP A0A3F2YLZ0
B	346	HIS	-	expression tag	UNP A0A3F2YLZ0
B	347	HIS	-	expression tag	UNP A0A3F2YLZ0
B	348	ASP	-	expression tag	UNP A0A3F2YLZ0
B	349	TYR	-	expression tag	UNP A0A3F2YLZ0
B	350	LYS	-	expression tag	UNP A0A3F2YLZ0
B	351	ASP	-	expression tag	UNP A0A3F2YLZ0
B	352	ASP	-	expression tag	UNP A0A3F2YLZ0
B	353	ASP	-	expression tag	UNP A0A3F2YLZ0
B	354	ASP	-	expression tag	UNP A0A3F2YLZ0
B	355	LYS	-	expression tag	UNP A0A3F2YLZ0
C	1	MET	-	initiating methionine	UNP A0A3F2YLZ0
C	334	ALA	-	expression tag	UNP A0A3F2YLZ0
C	335	GLU	-	expression tag	UNP A0A3F2YLZ0
C	336	ASN	-	expression tag	UNP A0A3F2YLZ0
C	337	LEU	-	expression tag	UNP A0A3F2YLZ0
C	338	TYR	-	expression tag	UNP A0A3F2YLZ0
C	339	PHE	-	expression tag	UNP A0A3F2YLZ0
C	340	GLN	-	expression tag	UNP A0A3F2YLZ0
C	341	SER	-	expression tag	UNP A0A3F2YLZ0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	342	HIS	-	expression tag	UNP A0A3F2YLZ0
C	343	HIS	-	expression tag	UNP A0A3F2YLZ0
C	344	HIS	-	expression tag	UNP A0A3F2YLZ0
C	345	HIS	-	expression tag	UNP A0A3F2YLZ0
C	346	HIS	-	expression tag	UNP A0A3F2YLZ0
C	347	HIS	-	expression tag	UNP A0A3F2YLZ0
C	348	ASP	-	expression tag	UNP A0A3F2YLZ0
C	349	TYR	-	expression tag	UNP A0A3F2YLZ0
C	350	LYS	-	expression tag	UNP A0A3F2YLZ0
C	351	ASP	-	expression tag	UNP A0A3F2YLZ0
C	352	ASP	-	expression tag	UNP A0A3F2YLZ0
C	353	ASP	-	expression tag	UNP A0A3F2YLZ0
C	354	ASP	-	expression tag	UNP A0A3F2YLZ0
C	355	LYS	-	expression tag	UNP A0A3F2YLZ0
D	1	MET	-	initiating methionine	UNP A0A3F2YLZ0
D	334	ALA	-	expression tag	UNP A0A3F2YLZ0
D	335	GLU	-	expression tag	UNP A0A3F2YLZ0
D	336	ASN	-	expression tag	UNP A0A3F2YLZ0
D	337	LEU	-	expression tag	UNP A0A3F2YLZ0
D	338	TYR	-	expression tag	UNP A0A3F2YLZ0
D	339	PHE	-	expression tag	UNP A0A3F2YLZ0
D	340	GLN	-	expression tag	UNP A0A3F2YLZ0
D	341	SER	-	expression tag	UNP A0A3F2YLZ0
D	342	HIS	-	expression tag	UNP A0A3F2YLZ0
D	343	HIS	-	expression tag	UNP A0A3F2YLZ0
D	344	HIS	-	expression tag	UNP A0A3F2YLZ0
D	345	HIS	-	expression tag	UNP A0A3F2YLZ0
D	346	HIS	-	expression tag	UNP A0A3F2YLZ0
D	347	HIS	-	expression tag	UNP A0A3F2YLZ0
D	348	ASP	-	expression tag	UNP A0A3F2YLZ0
D	349	TYR	-	expression tag	UNP A0A3F2YLZ0
D	350	LYS	-	expression tag	UNP A0A3F2YLZ0
D	351	ASP	-	expression tag	UNP A0A3F2YLZ0
D	352	ASP	-	expression tag	UNP A0A3F2YLZ0
D	353	ASP	-	expression tag	UNP A0A3F2YLZ0
D	354	ASP	-	expression tag	UNP A0A3F2YLZ0
D	355	LYS	-	expression tag	UNP A0A3F2YLZ0
E	1	MET	-	initiating methionine	UNP A0A3F2YLZ0
E	334	ALA	-	expression tag	UNP A0A3F2YLZ0
E	335	GLU	-	expression tag	UNP A0A3F2YLZ0
E	336	ASN	-	expression tag	UNP A0A3F2YLZ0
E	337	LEU	-	expression tag	UNP A0A3F2YLZ0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	338	TYR	-	expression tag	UNP A0A3F2YLZ0
E	339	PHE	-	expression tag	UNP A0A3F2YLZ0
E	340	GLN	-	expression tag	UNP A0A3F2YLZ0
E	341	SER	-	expression tag	UNP A0A3F2YLZ0
E	342	HIS	-	expression tag	UNP A0A3F2YLZ0
E	343	HIS	-	expression tag	UNP A0A3F2YLZ0
E	344	HIS	-	expression tag	UNP A0A3F2YLZ0
E	345	HIS	-	expression tag	UNP A0A3F2YLZ0
E	346	HIS	-	expression tag	UNP A0A3F2YLZ0
E	347	HIS	-	expression tag	UNP A0A3F2YLZ0
E	348	ASP	-	expression tag	UNP A0A3F2YLZ0
E	349	TYR	-	expression tag	UNP A0A3F2YLZ0
E	350	LYS	-	expression tag	UNP A0A3F2YLZ0
E	351	ASP	-	expression tag	UNP A0A3F2YLZ0
E	352	ASP	-	expression tag	UNP A0A3F2YLZ0
E	353	ASP	-	expression tag	UNP A0A3F2YLZ0
E	354	ASP	-	expression tag	UNP A0A3F2YLZ0
E	355	LYS	-	expression tag	UNP A0A3F2YLZ0
F	1	MET	-	initiating methionine	UNP A0A3F2YLZ0
F	334	ALA	-	expression tag	UNP A0A3F2YLZ0
F	335	GLU	-	expression tag	UNP A0A3F2YLZ0
F	336	ASN	-	expression tag	UNP A0A3F2YLZ0
F	337	LEU	-	expression tag	UNP A0A3F2YLZ0
F	338	TYR	-	expression tag	UNP A0A3F2YLZ0
F	339	PHE	-	expression tag	UNP A0A3F2YLZ0
F	340	GLN	-	expression tag	UNP A0A3F2YLZ0
F	341	SER	-	expression tag	UNP A0A3F2YLZ0
F	342	HIS	-	expression tag	UNP A0A3F2YLZ0
F	343	HIS	-	expression tag	UNP A0A3F2YLZ0
F	344	HIS	-	expression tag	UNP A0A3F2YLZ0
F	345	HIS	-	expression tag	UNP A0A3F2YLZ0
F	346	HIS	-	expression tag	UNP A0A3F2YLZ0
F	347	HIS	-	expression tag	UNP A0A3F2YLZ0
F	348	ASP	-	expression tag	UNP A0A3F2YLZ0
F	349	TYR	-	expression tag	UNP A0A3F2YLZ0
F	350	LYS	-	expression tag	UNP A0A3F2YLZ0
F	351	ASP	-	expression tag	UNP A0A3F2YLZ0
F	352	ASP	-	expression tag	UNP A0A3F2YLZ0
F	353	ASP	-	expression tag	UNP A0A3F2YLZ0
F	354	ASP	-	expression tag	UNP A0A3F2YLZ0
F	355	LYS	-	expression tag	UNP A0A3F2YLZ0
G	1	MET	-	initiating methionine	UNP A0A3F2YLZ0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	334	ALA	-	expression tag	UNP A0A3F2YLZ0
G	335	GLU	-	expression tag	UNP A0A3F2YLZ0
G	336	ASN	-	expression tag	UNP A0A3F2YLZ0
G	337	LEU	-	expression tag	UNP A0A3F2YLZ0
G	338	TYR	-	expression tag	UNP A0A3F2YLZ0
G	339	PHE	-	expression tag	UNP A0A3F2YLZ0
G	340	GLN	-	expression tag	UNP A0A3F2YLZ0
G	341	SER	-	expression tag	UNP A0A3F2YLZ0
G	342	HIS	-	expression tag	UNP A0A3F2YLZ0
G	343	HIS	-	expression tag	UNP A0A3F2YLZ0
G	344	HIS	-	expression tag	UNP A0A3F2YLZ0
G	345	HIS	-	expression tag	UNP A0A3F2YLZ0
G	346	HIS	-	expression tag	UNP A0A3F2YLZ0
G	347	HIS	-	expression tag	UNP A0A3F2YLZ0
G	348	ASP	-	expression tag	UNP A0A3F2YLZ0
G	349	TYR	-	expression tag	UNP A0A3F2YLZ0
G	350	LYS	-	expression tag	UNP A0A3F2YLZ0
G	351	ASP	-	expression tag	UNP A0A3F2YLZ0
G	352	ASP	-	expression tag	UNP A0A3F2YLZ0
G	353	ASP	-	expression tag	UNP A0A3F2YLZ0
G	354	ASP	-	expression tag	UNP A0A3F2YLZ0
G	355	LYS	-	expression tag	UNP A0A3F2YLZ0
H	1	MET	-	initiating methionine	UNP A0A3F2YLZ0
H	334	ALA	-	expression tag	UNP A0A3F2YLZ0
H	335	GLU	-	expression tag	UNP A0A3F2YLZ0
H	336	ASN	-	expression tag	UNP A0A3F2YLZ0
H	337	LEU	-	expression tag	UNP A0A3F2YLZ0
H	338	TYR	-	expression tag	UNP A0A3F2YLZ0
H	339	PHE	-	expression tag	UNP A0A3F2YLZ0
H	340	GLN	-	expression tag	UNP A0A3F2YLZ0
H	341	SER	-	expression tag	UNP A0A3F2YLZ0
H	342	HIS	-	expression tag	UNP A0A3F2YLZ0
H	343	HIS	-	expression tag	UNP A0A3F2YLZ0
H	344	HIS	-	expression tag	UNP A0A3F2YLZ0
H	345	HIS	-	expression tag	UNP A0A3F2YLZ0
H	346	HIS	-	expression tag	UNP A0A3F2YLZ0
H	347	HIS	-	expression tag	UNP A0A3F2YLZ0
H	348	ASP	-	expression tag	UNP A0A3F2YLZ0
H	349	TYR	-	expression tag	UNP A0A3F2YLZ0
H	350	LYS	-	expression tag	UNP A0A3F2YLZ0
H	351	ASP	-	expression tag	UNP A0A3F2YLZ0
H	352	ASP	-	expression tag	UNP A0A3F2YLZ0

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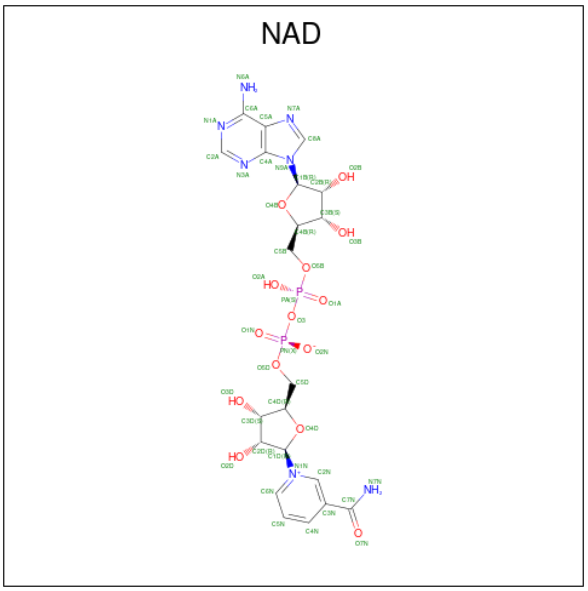
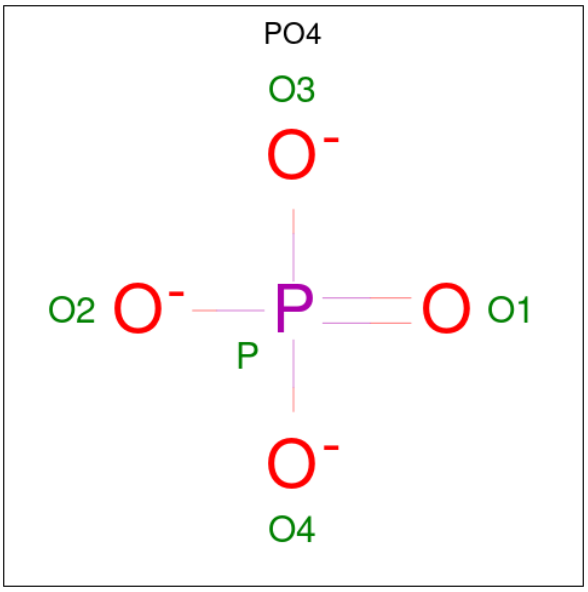
Chain	Residue	Modelled	Actual	Comment	Reference
H	353	ASP	-	expression tag	UNP A0A3F2YLZ0
H	354	ASP	-	expression tag	UNP A0A3F2YLZ0
H	355	LYS	-	expression tag	UNP A0A3F2YLZ0

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	H	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	23	Total O 23 23	0	0
4	B	15	Total O 15 15	0	0
4	C	35	Total O 35 35	0	0
4	D	34	Total O 34 34	0	0

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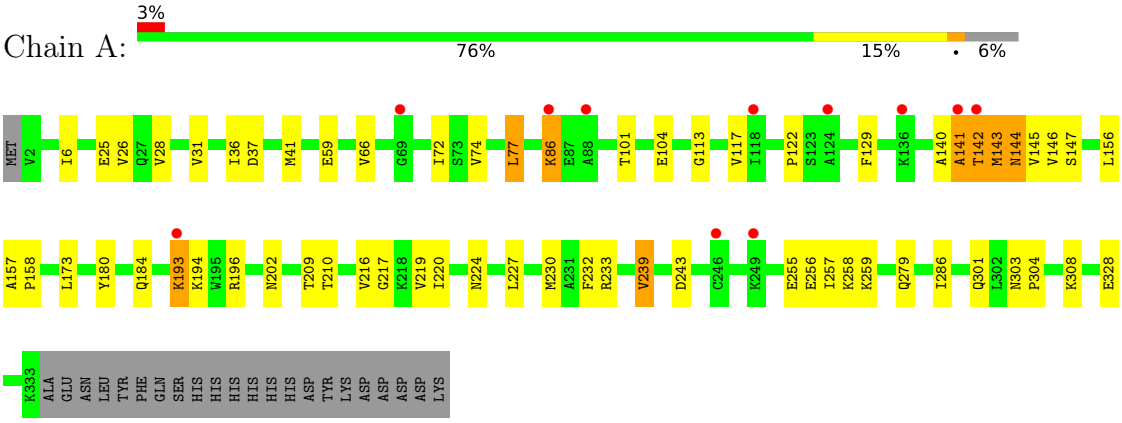
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	29	Total O 29 29	0	0
4	F	19	Total O 19 19	0	0
4	G	20	Total O 20 20	0	0
4	H	48	Total O 48 48	0	0

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.

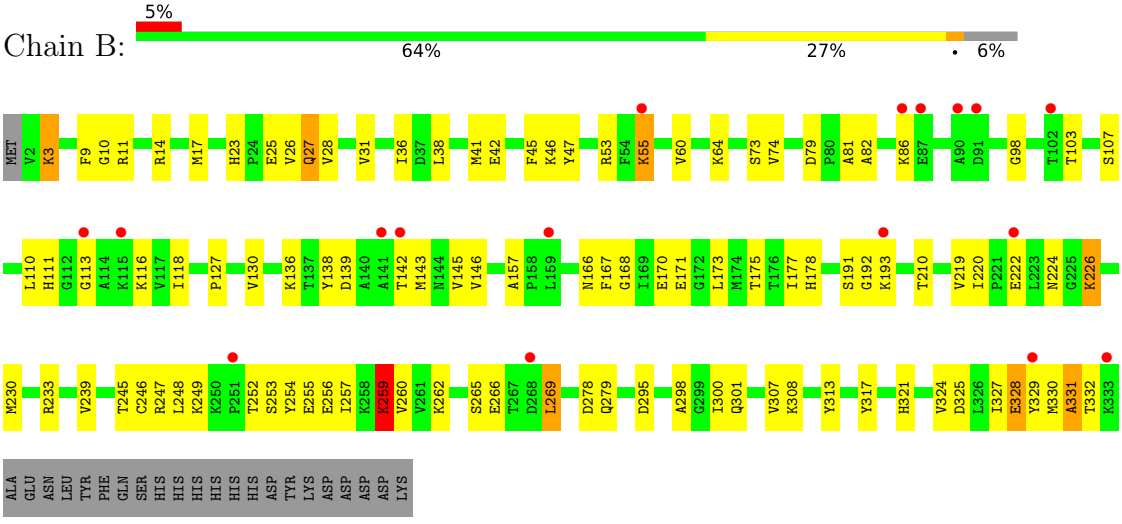
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:



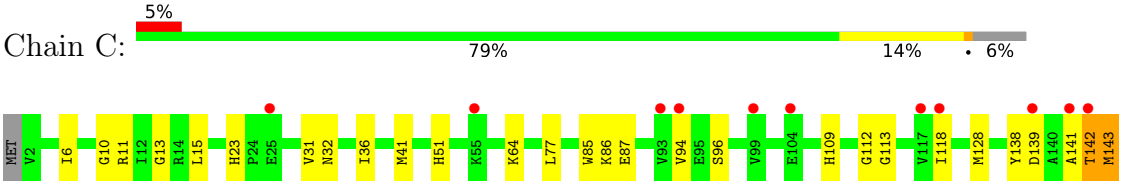
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

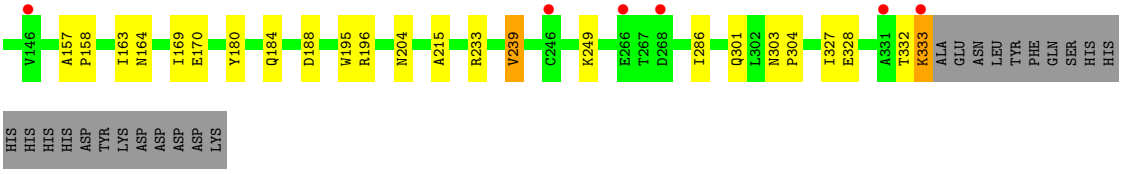
Chain B:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

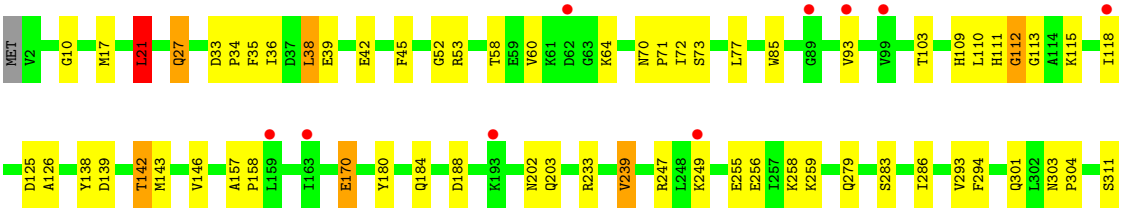
Chain C:

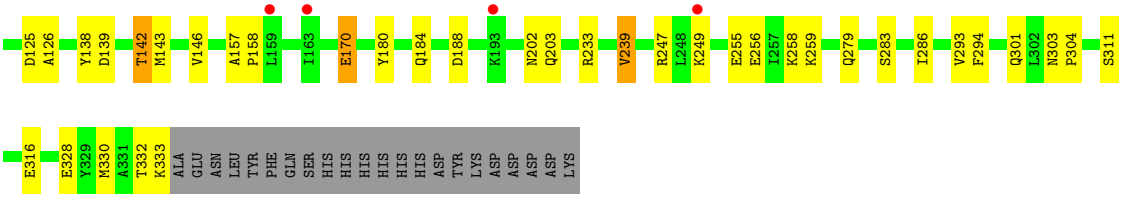




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

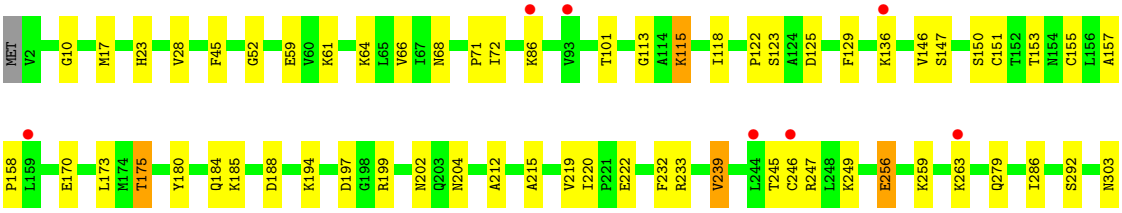
Chain D:

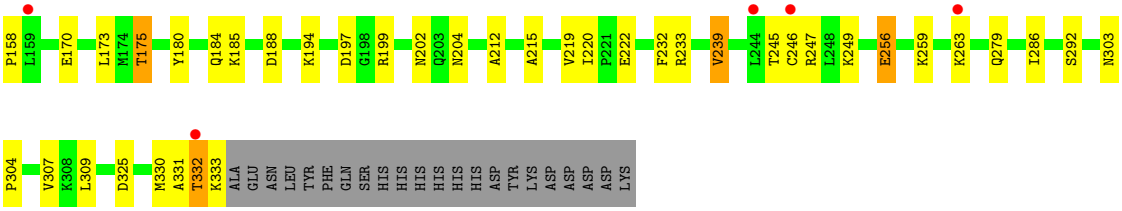




• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

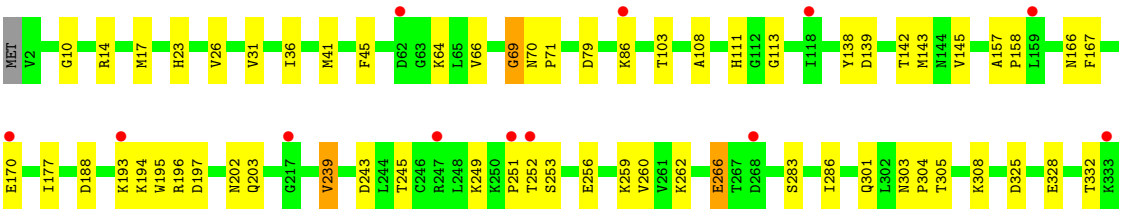
Chain E:





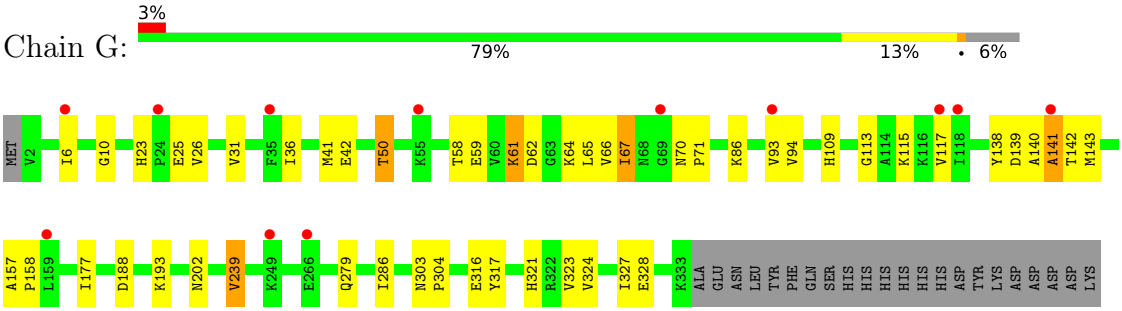
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain F:



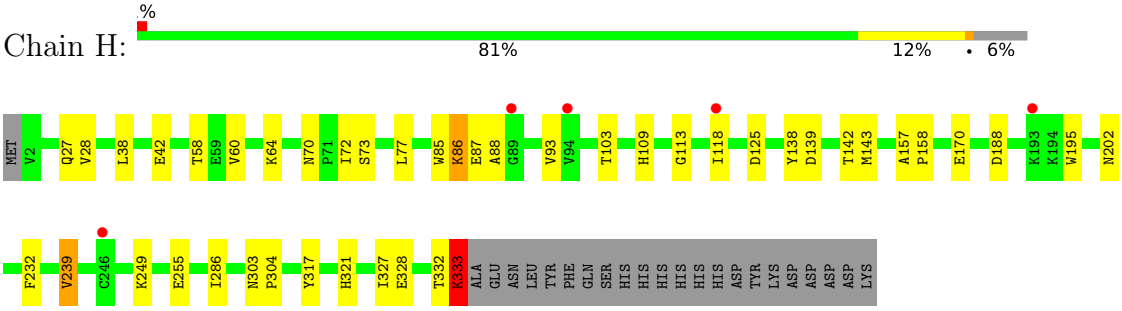
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain G:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.22Å 79.12Å 138.82Å 76.68° 77.70° 67.98°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 1.95	Depositor EDS
% Data completeness (in resolution range)	78.9 (19.95-2.40) 63.3 (19.95-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.63 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.209 , 0.232 0.210 , 0.232	Depositor DCC
R_{free} test set	8003 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20862	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.54	2/2583 (0.1%)	0.72	3/3506 (0.1%)
1	B	0.56	1/2582 (0.0%)	0.78	9/3504 (0.3%)
1	C	0.47	0/2583	0.66	3/3506 (0.1%)
1	D	0.49	0/2583	0.71	3/3506 (0.1%)
1	E	0.53	0/2583	0.70	2/3506 (0.1%)
1	F	0.49	0/2583	0.71	5/3506 (0.1%)
1	G	0.48	0/2583	0.65	1/3506 (0.0%)
1	H	0.51	1/2583 (0.0%)	0.67	1/3506 (0.0%)
All	All	0.51	4/20663 (0.0%)	0.70	27/28046 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	GLU	CG-CD	-11.16	1.35	1.51
1	A	104	GLU	CD-OE2	7.35	1.33	1.25
1	H	333	LYS	CA-C	6.28	1.69	1.52
1	A	104	GLU	CD-OE1	5.68	1.31	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	27	GLN	CA-CB-CG	-11.00	89.20	113.40
1	B	247	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	D	112	GLY	N-CA-C	-8.45	91.97	113.10
1	F	69	GLY	N-CA-C	-8.05	92.97	113.10
1	B	259	LYS	CD-CE-NZ	-7.47	94.51	111.70
1	B	259	LYS	CG-CD-CE	7.35	133.94	111.90
1	B	259	LYS	CA-CB-CG	6.83	128.42	113.40
1	F	79	ASP	CB-CG-OD1	-6.55	112.40	118.30
1	B	222	GLU	CA-CB-CG	6.46	127.62	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	21	LEU	CB-CG-CD1	6.01	121.21	111.00
1	A	143	MET	N-CA-C	5.90	126.93	111.00
1	B	55	LYS	CA-CB-CG	-5.76	100.73	113.40
1	D	188	ASP	CB-CG-OD1	5.76	123.48	118.30
1	F	79	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	188	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	256	GLU	CB-CA-C	5.66	121.71	110.40
1	G	188	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	196	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	F	196	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	F	188	ASP	CB-CG-OD1	5.57	123.32	118.30
1	H	188	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	144	ASN	N-CA-C	5.36	125.47	111.00
1	B	255	GLU	CA-CB-CG	-5.32	101.69	113.40
1	E	188	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	269	LEU	CA-CB-CG	-5.26	103.19	115.30
1	A	37	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	64	LYS	CD-CE-NZ	5.06	123.33	111.70

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	2531	0	2534	85	0
1	B	2530	0	2533	90	0
1	C	2531	0	2534	69	0
1	D	2531	0	2534	77	0
1	E	2531	0	2534	82	0
1	F	2531	0	2534	61	0
1	G	2531	0	2534	48	0
1	H	2531	0	2534	40	0
2	A	44	0	26	2	0
2	B	44	0	26	3	0
2	C	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	26	5	0
2	E	44	0	26	2	0
2	F	44	0	26	0	0
2	G	44	0	26	2	0
2	H	44	0	26	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	23	0	0	26	0
4	B	15	0	0	20	0
4	C	35	0	0	16	0
4	D	34	0	0	26	0
4	E	29	0	0	23	0
4	F	19	0	0	3	0
4	G	20	0	0	8	0
4	H	48	0	0	9	0
All	All	20862	0	20479	525	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 13.

All (525) 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:H:333:LYS:HD2	4:H:502:HOH:O	1.11	1.28
1:E:292:SER:HB2	4:E:504:HOH:O	1.30	1.27
1:C:139:ASP:H	1:C:143:MET:CE	1.47	1.26
1:E:155:CYS:HA	4:E:504:HOH:O	1.37	1.23
1:C:141:ALA:CA	4:C:501:HOH:O	1.88	1.20
1:F:66:VAL:CG1	1:F:69:GLY:O	1.94	1.14
1:C:142:THR:N	4:C:501:HOH:O	1.80	1.13
1:D:294:PHE:HA	4:D:502:HOH:O	1.45	1.12
1:C:141:ALA:HB3	4:C:501:HOH:O	1.48	1.12
1:E:331:ALA:O	1:E:332:THR:OG1	1.67	1.11
1:A:308:LYS:NZ	4:A:502:HOH:O	1.84	1.09
1:E:17:MET:SD	1:E:28:VAL:HG21	1.94	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ASN:N	4:E:502:HOH:O	1.88	1.07
1:B:191:SER:C	4:B:502:HOH:O	1.93	1.07
1:C:139:ASP:H	1:C:143:MET:HE1	0.97	1.06
1:E:219:VAL:HG23	1:E:220:ILE:HD12	1.37	1.06
1:A:26:VAL:CG2	4:A:505:HOH:O	2.05	1.05
1:A:26:VAL:N	4:A:505:HOH:O	1.87	1.04
1:C:139:ASP:N	1:C:143:MET:HE1	1.71	1.04
1:A:219:VAL:HG23	1:A:220:ILE:HD12	1.37	1.03
1:F:66:VAL:HG13	1:F:69:GLY:O	1.56	1.02
1:H:317:TYR:CZ	4:H:505:HOH:O	2.14	1.00
1:A:26:VAL:CA	4:A:505:HOH:O	2.09	1.00
1:G:59:GLU:HA	4:G:504:HOH:O	1.59	1.00
1:C:13:GLY:CA	4:C:503:HOH:O	2.09	1.00
1:B:278:ASP:O	4:B:501:HOH:O	1.81	0.98
1:C:13:GLY:N	4:C:503:HOH:O	1.96	0.98
1:A:258:LYS:N	4:A:506:HOH:O	1.96	0.97
2:A:401:NAD:O2A	4:A:501:HOH:O	1.81	0.97
1:C:139:ASP:N	1:C:143:MET:CE	2.26	0.95
1:F:66:VAL:HG12	1:F:69:GLY:O	1.66	0.95
1:A:193:LYS:O	4:A:503:HOH:O	1.85	0.94
1:A:279:GLN:OE1	4:A:504:HOH:O	1.85	0.94
1:E:125:ASP:OD1	4:E:501:HOH:O	1.83	0.93
1:E:123:SER:OG	4:E:501:HOH:O	1.85	0.93
1:D:17:MET:O	1:D:21:LEU:HD13	1.68	0.93
1:D:316:GLU:OE2	4:D:501:HOH:O	1.86	0.93
1:A:202:ASN:ND2	1:D:202:ASN:CG	2.22	0.92
1:F:70:ASN:OD1	4:F:501:HOH:O	1.88	0.92
1:E:153:THR:HG22	1:E:212:ALA:HA	1.52	0.91
1:C:139:ASP:O	4:C:502:HOH:O	1.88	0.91
1:A:193:LYS:C	4:A:503:HOH:O	2.08	0.91
1:E:175:THR:HG21	1:F:243:ASP:OD2	1.72	0.90
1:A:59:GLU:HB3	1:A:66:VAL:CG1	2.03	0.89
1:B:27:GLN:HG3	1:B:28:VAL:N	1.87	0.89
1:D:35:PHE:C	1:D:36:ILE:HD12	1.93	0.88
2:E:401:NAD:O2A	4:E:503:HOH:O	1.90	0.88
1:E:59:GLU:HB3	1:E:66:VAL:CG1	2.03	0.88
1:E:292:SER:CB	4:E:504:HOH:O	2.00	0.87
1:F:70:ASN:CG	4:F:501:HOH:O	2.12	0.87
1:A:256:GLU:C	4:A:506:HOH:O	2.10	0.87
1:D:311:SER:OG	4:D:502:HOH:O	1.92	0.87
1:C:13:GLY:HA3	4:C:503:HOH:O	1.69	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:NAD:N7A	4:B:504:HOH:O	2.08	0.86
1:F:103:THR:HG23	1:F:145:VAL:HG21	1.54	0.86
1:F:167:PHE:CE1	1:F:252:THR:HG21	2.10	0.86
1:B:82:ALA:N	4:B:503:HOH:O	2.06	0.86
1:B:25:GLU:OE2	1:B:328:GLU:OE2	1.93	0.85
1:C:32:ASN:HD21	1:C:77:LEU:H	1.21	0.85
1:D:311:SER:CB	4:D:502:HOH:O	2.23	0.85
1:B:210:THR:HG21	4:B:505:HOH:O	1.76	0.85
1:H:332:THR:C	4:H:502:HOH:O	2.14	0.85
1:D:203:GLN:HG3	4:D:511:HOH:O	1.75	0.85
1:F:70:ASN:ND2	4:F:501:HOH:O	2.08	0.85
1:G:193:LYS:O	4:G:501:HOH:O	1.93	0.85
1:B:192:GLY:N	4:B:502:HOH:O	2.04	0.84
1:C:141:ALA:N	4:C:501:HOH:O	1.94	0.84
1:E:245:THR:CA	4:E:505:HOH:O	2.25	0.84
1:C:141:ALA:CB	4:C:501:HOH:O	1.97	0.84
1:H:28:VAL:O	1:H:72:ILE:CD1	2.26	0.84
1:A:28:VAL:O	1:A:72:ILE:CD1	2.27	0.83
2:D:401:NAD:C4A	4:D:503:HOH:O	2.25	0.83
1:B:79:ASP:CG	4:B:503:HOH:O	2.17	0.83
1:F:202:ASN:CG	1:G:202:ASN:OD1	2.16	0.82
1:G:316:GLU:OE2	4:G:502:HOH:O	1.98	0.82
1:D:294:PHE:CA	4:D:502:HOH:O	2.14	0.82
1:E:155:CYS:O	4:E:504:HOH:O	1.97	0.82
1:D:139:ASP:OD1	4:D:504:HOH:O	1.98	0.81
1:F:64:LYS:HE2	1:F:71:PRO:HB2	1.63	0.81
1:D:113:GLY:N	4:D:505:HOH:O	2.03	0.81
1:F:202:ASN:OD1	1:G:202:ASN:CG	2.19	0.81
1:C:139:ASP:H	1:C:143:MET:HE2	1.44	0.81
1:D:33:ASP:OD1	4:D:503:HOH:O	1.98	0.81
1:E:245:THR:HA	4:E:505:HOH:O	1.81	0.80
1:G:70:ASN:OD1	4:G:503:HOH:O	1.99	0.80
1:H:332:THR:O	4:H:502:HOH:O	1.99	0.79
1:E:155:CYS:CA	4:E:504:HOH:O	2.10	0.79
1:H:255:GLU:OE2	4:H:503:HOH:O	2.00	0.78
1:A:202:ASN:HD21	1:D:202:ASN:ND2	1.82	0.77
1:H:118:ILE:HD12	1:H:327:ILE:HG13	1.67	0.77
1:A:117:VAL:CG1	1:A:145:VAL:HG22	2.15	0.77
2:D:401:NAD:N3A	4:D:503:HOH:O	2.18	0.77
1:A:255:GLU:O	4:A:506:HOH:O	2.02	0.76
1:A:117:VAL:HG12	1:A:145:VAL:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:O	1:B:55:LYS:NZ	2.19	0.76
1:C:118:ILE:HD12	1:C:327:ILE:HG13	1.68	0.76
1:E:307:VAL:O	4:E:505:HOH:O	2.03	0.76
1:C:10:GLY:N	4:C:503:HOH:O	2.19	0.75
1:G:138:TYR:HA	1:G:143:MET:HE1	1.68	0.75
1:A:202:ASN:CG	1:D:202:ASN:OD1	2.25	0.75
1:H:138:TYR:HA	1:H:143:MET:HE1	1.67	0.75
1:A:259:LYS:N	4:A:506:HOH:O	1.88	0.75
1:D:138:TYR:HA	1:D:143:MET:HE1	1.68	0.75
1:F:138:TYR:HA	1:F:143:MET:HE1	1.67	0.74
1:H:328:GLU:OE2	4:H:504:HOH:O	2.05	0.74
1:A:156:LEU:HD21	1:A:227:LEU:HD11	1.67	0.74
1:G:139:ASP:HB3	1:G:142:THR:HG22	1.69	0.74
1:C:109:HIS:O	4:C:504:HOH:O	2.04	0.73
1:B:25:GLU:HG2	1:B:26:VAL:N	2.03	0.73
1:E:64:LYS:HE2	1:E:71:PRO:HB2	1.70	0.73
1:A:217:GLY:HA3	1:A:224:ASN:HD22	1.52	0.73
1:G:64:LYS:HE2	1:G:71:PRO:HB2	1.70	0.73
1:B:25:GLU:HG2	1:B:26:VAL:H	1.52	0.72
1:E:245:THR:HB	4:E:505:HOH:O	1.89	0.72
2:D:401:NAD:H1B	4:D:503:HOH:O	1.88	0.71
1:F:170:GLU:HG3	1:F:249:LYS:HG2	1.73	0.71
1:C:139:ASP:OD2	4:C:501:HOH:O	2.09	0.70
1:H:87:GLU:O	1:H:88:ALA:HB3	1.90	0.70
1:C:138:TYR:HA	1:C:143:MET:HE1	1.72	0.70
1:G:58:THR:O	4:G:504:HOH:O	2.09	0.70
1:A:140:ALA:O	1:A:141:ALA:CB	2.40	0.70
1:G:140:ALA:O	1:G:141:ALA:CB	2.39	0.70
1:A:216:VAL:HG11	1:A:227:LEU:HD12	1.73	0.70
1:B:166:ASN:OD1	1:B:260:VAL:HG21	1.92	0.70
1:G:324:VAL:O	1:G:327:ILE:HG12	1.92	0.70
1:A:255:GLU:OE1	4:A:508:HOH:O	2.09	0.69
1:G:323:VAL:O	1:G:327:ILE:HG23	1.92	0.69
1:D:118:ILE:HD11	1:D:330:MET:SD	2.31	0.69
1:H:139:ASP:HB3	1:H:142:THR:HG22	1.73	0.69
1:C:96:SER:O	4:C:505:HOH:O	2.09	0.69
1:B:170:GLU:OE2	1:B:249:LYS:HB2	1.92	0.69
1:E:151:CYS:O	4:E:506:HOH:O	2.11	0.69
1:E:331:ALA:O	1:E:332:THR:CB	2.41	0.68
1:F:166:ASN:ND2	1:F:260:VAL:HG21	2.08	0.68
1:A:202:ASN:ND2	1:D:202:ASN:ND2	2.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:ALA:O	1:G:141:ALA:HB3	1.93	0.68
1:A:140:ALA:O	1:A:141:ALA:HB3	1.94	0.68
1:B:193:LYS:N	4:B:502:HOH:O	1.90	0.68
1:C:333:LYS:CD	1:C:333:LYS:H	2.06	0.67
1:D:112:GLY:CA	4:D:505:HOH:O	2.40	0.67
1:A:129:PHE:HD2	1:A:146:VAL:CG2	2.07	0.67
1:H:28:VAL:O	1:H:72:ILE:HD12	1.93	0.67
1:A:129:PHE:CD2	1:A:146:VAL:CG2	2.78	0.67
1:E:129:PHE:HD2	1:E:146:VAL:CG2	2.06	0.67
1:F:142:THR:HG23	1:F:143:MET:HG3	1.77	0.67
1:A:25:GLU:C	4:A:505:HOH:O	2.27	0.66
1:F:139:ASP:HB3	1:F:142:THR:HG22	1.77	0.66
1:E:129:PHE:CD2	1:E:146:VAL:CG2	2.78	0.66
1:C:333:LYS:CD	1:C:333:LYS:N	2.58	0.66
1:G:279:GLN:HE21	1:H:195:TRP:HB2	1.60	0.65
1:D:328:GLU:OE2	4:D:507:HOH:O	2.12	0.65
1:F:252:THR:OG1	1:F:256:GLU:OE1	2.09	0.65
1:C:10:GLY:HA3	2:C:401:NAD:O5B	1.97	0.64
1:B:79:ASP:CB	4:B:503:HOH:O	2.44	0.64
1:B:230:MET:O	4:B:505:HOH:O	2.14	0.64
1:C:51:HIS:O	4:C:506:HOH:O	2.14	0.64
1:F:202:ASN:ND2	1:G:202:ASN:OD1	2.30	0.64
1:G:327:ILE:HG13	1:G:328:GLU:N	2.12	0.64
1:A:184:GLN:HB3	4:A:516:HOH:O	1.98	0.64
1:G:50:THR:HG21	4:G:505:HOH:O	1.97	0.64
1:D:70:ASN:O	1:D:72:ILE:HD12	1.99	0.63
1:A:26:VAL:HG23	4:A:505:HOH:O	1.81	0.63
1:E:153:THR:HG22	1:E:212:ALA:CA	2.27	0.63
1:D:170:GLU:OE1	1:D:249:LYS:HG2	1.99	0.63
1:A:184:GLN:HE21	1:A:233:ARG:HH11	1.47	0.63
1:A:28:VAL:O	1:A:72:ILE:HD12	1.99	0.62
1:D:294:PHE:N	4:D:502:HOH:O	2.31	0.62
1:F:167:PHE:CD1	1:F:252:THR:HG21	2.35	0.62
1:A:230:MET:HE2	1:B:308:LYS:HD2	1.81	0.62
1:F:23:HIS:HE1	1:F:325:ASP:OD1	1.82	0.62
1:E:153:THR:CG2	1:E:212:ALA:HA	2.28	0.62
1:G:61:LYS:HD3	1:G:62:ASP:OD2	2.00	0.62
1:C:164:ASN:HA	1:C:169:ILE:HD12	1.83	0.61
1:C:184:GLN:HE21	1:C:233:ARG:HH11	1.47	0.61
1:E:28:VAL:HG23	1:E:28:VAL:O	2.01	0.61
1:E:175:THR:CG2	1:F:243:ASP:OD2	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:GLN:HE21	1:E:233:ARG:HH11	1.48	0.61
1:G:10:GLY:HA3	2:G:401:NAD:O5B	2.00	0.61
1:F:166:ASN:CG	1:F:260:VAL:HG21	2.20	0.61
1:C:139:ASP:N	1:C:143:MET:HE2	2.08	0.61
1:D:142:THR:HG22	1:D:143:MET:HG3	1.82	0.61
1:A:230:MET:HB3	1:B:300:ILE:HD11	1.83	0.60
1:F:202:ASN:OD1	1:G:202:ASN:ND2	2.34	0.60
1:B:79:ASP:O	4:B:503:HOH:O	2.16	0.60
1:E:118:ILE:HD11	1:E:330:MET:SD	2.42	0.60
1:B:230:MET:N	4:B:505:HOH:O	2.35	0.60
1:A:101:THR:HG23	1:A:122:PRO:O	2.01	0.60
1:A:216:VAL:HG11	1:A:227:LEU:CD1	2.31	0.60
1:C:138:TYR:CD1	1:C:143:MET:HE3	2.37	0.59
1:A:59:GLU:HB3	1:A:66:VAL:HG13	1.85	0.59
1:B:167:PHE:CB	1:B:248:LEU:HD23	2.32	0.59
1:A:59:GLU:O	1:A:66:VAL:HG12	2.03	0.59
1:E:59:GLU:O	1:E:66:VAL:HG12	2.02	0.59
1:E:101:THR:HG23	1:E:122:PRO:O	2.03	0.59
1:E:129:PHE:CD2	1:E:146:VAL:HG21	2.38	0.59
1:H:142:THR:HG23	1:H:143:MET:HG3	1.85	0.59
1:A:143:MET:O	1:A:145:VAL:N	2.36	0.59
1:D:184:GLN:HE21	1:D:233:ARG:HH11	1.48	0.59
1:B:167:PHE:HB3	1:B:248:LEU:HD23	1.85	0.58
1:E:194:LYS:NZ	1:E:197:ASP:OD2	2.27	0.58
1:H:64:LYS:NZ	1:H:73:SER:OG	2.36	0.58
1:A:196:ARG:NH2	1:B:295:ASP:OD2	2.37	0.58
1:E:129:PHE:CD2	1:E:146:VAL:HG23	2.38	0.58
1:B:245:THR:HG22	1:B:308:LYS:HG3	1.84	0.58
1:C:138:TYR:HA	1:C:143:MET:CE	2.33	0.58
1:D:111:HIS:C	1:D:112:GLY:O	2.39	0.58
1:A:26:VAL:HG22	4:A:505:HOH:O	1.85	0.58
1:A:129:PHE:CD2	1:A:146:VAL:HG21	2.38	0.57
1:E:150:SER:OG	1:E:153:THR:HG23	2.04	0.57
1:D:103:THR:HG23	1:D:125:ASP:OD1	2.04	0.57
1:D:64:LYS:NZ	1:D:73:SER:OG	2.37	0.57
1:D:33:ASP:CG	1:D:36:ILE:HD13	2.24	0.57
1:B:262:LYS:O	1:B:266:GLU:HG3	2.05	0.57
1:H:103:THR:HG23	1:H:125:ASP:OD1	2.04	0.57
1:D:112:GLY:HA2	4:D:505:HOH:O	2.04	0.57
1:A:129:PHE:CD2	1:A:146:VAL:HG23	2.39	0.57
1:F:103:THR:HG23	1:F:145:VAL:CG2	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:TYR:OH	4:H:505:HOH:O	2.11	0.56
1:D:52:GLY:CA	4:D:509:HOH:O	2.53	0.56
1:E:202:ASN:OD1	1:H:202:ASN:OD1	2.24	0.56
1:D:33:ASP:CG	4:D:503:HOH:O	2.43	0.56
1:D:70:ASN:O	1:D:72:ILE:CD1	2.53	0.56
1:D:38:LEU:HD13	1:D:38:LEU:C	2.26	0.56
1:E:10:GLY:HA3	2:E:401:NAD:O5B	2.06	0.56
1:A:303:ASN:ND2	1:B:171:GLU:OE2	2.39	0.56
1:C:333:LYS:N	1:C:333:LYS:HD2	2.21	0.56
1:F:249:LYS:O	1:F:251:PRO:HD3	2.06	0.56
1:B:253:SER:O	1:B:257:ILE:HG13	2.06	0.55
1:C:118:ILE:HD12	1:C:327:ILE:CG1	2.35	0.55
1:H:138:TYR:OH	4:H:501:HOH:O	1.99	0.55
1:G:138:TYR:CD1	1:G:143:MET:CE	2.90	0.55
1:H:138:TYR:CD1	1:H:143:MET:CE	2.90	0.55
1:C:138:TYR:CA	1:C:143:MET:HE1	2.36	0.55
1:D:118:ILE:HD13	1:D:146:VAL:HG22	1.89	0.55
1:C:31:VAL:HG11	1:C:41:MET:HE3	1.87	0.55
1:D:33:ASP:OD1	1:D:36:ILE:HD13	2.07	0.55
1:H:60:VAL:HG22	4:H:518:HOH:O	2.06	0.55
1:D:138:TYR:CD1	1:D:143:MET:CE	2.90	0.55
1:B:219:VAL:HG23	1:B:220:ILE:HG13	1.89	0.55
2:D:401:NAD:C1B	4:D:503:HOH:O	2.50	0.55
1:E:59:GLU:OE2	1:E:61:LYS:HE3	2.05	0.55
1:E:309:LEU:N	1:E:309:LEU:HD12	2.22	0.55
1:F:138:TYR:CD1	1:F:143:MET:CE	2.90	0.55
1:B:38:LEU:HG	1:B:60:VAL:HG22	1.89	0.54
1:G:26:VAL:CG2	1:G:327:ILE:HD11	2.37	0.54
1:B:17:MET:HG2	1:B:45:PHE:CE1	2.43	0.54
1:F:31:VAL:HG11	1:F:41:MET:CE	2.38	0.54
1:F:203:GLN:OE1	1:G:50:THR:HG22	2.07	0.54
1:E:259:LYS:O	1:E:263:LYS:HG2	2.08	0.54
1:B:10:GLY:HA3	2:B:401:NAD:O5B	2.07	0.54
1:D:311:SER:HA	4:D:502:HOH:O	2.08	0.54
1:E:59:GLU:HB3	1:E:66:VAL:HG13	1.88	0.54
1:C:31:VAL:HG11	1:C:41:MET:CE	2.37	0.53
1:B:324:VAL:O	1:B:328:GLU:HG3	2.08	0.53
1:A:209:THR:HA	4:A:507:HOH:O	2.08	0.53
1:C:333:LYS:H	1:C:333:LYS:HD2	1.71	0.53
1:D:110:LEU:O	1:D:112:GLY:O	2.26	0.53
1:A:117:VAL:HG13	1:A:145:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LYS:HE3	1:B:138:TYR:OH	2.08	0.53
1:B:178:HIS:HB3	1:B:233:ARG:HD3	1.91	0.53
1:D:38:LEU:HD13	1:D:39:GLU:N	2.24	0.53
1:E:23:HIS:HE1	1:E:325:ASP:OD1	1.91	0.53
1:C:195:TRP:HB2	1:D:279:GLN:NE2	2.24	0.53
1:C:333:LYS:H	1:C:333:LYS:HD3	1.71	0.53
1:C:85:TRP:HD1	4:C:504:HOH:O	1.91	0.53
1:D:93:VAL:HG11	1:D:109:HIS:CD2	2.44	0.53
1:F:17:MET:HG2	1:F:45:PHE:CE1	2.44	0.53
1:A:26:VAL:HA	4:A:505:HOH:O	1.92	0.52
1:B:47:TYR:HA	4:B:510:HOH:O	2.07	0.52
1:B:136:LYS:HG2	1:B:329:TYR:OH	2.09	0.52
1:D:255:GLU:O	1:D:259:LYS:HG2	2.09	0.52
1:H:138:TYR:HD1	1:H:143:MET:CE	2.23	0.52
1:A:117:VAL:HG11	1:A:145:VAL:HG22	1.92	0.52
1:B:331:ALA:O	1:B:332:THR:HB	2.08	0.52
1:B:11:ARG:HH11	1:B:14:ARG:HH21	1.58	0.52
1:B:98:GLY:N	4:B:508:HOH:O	2.39	0.52
1:D:34:PRO:HD2	4:D:503:HOH:O	2.10	0.52
1:G:142:THR:HG23	1:G:143:MET:HG3	1.91	0.52
1:B:254:TYR:HD1	1:B:257:ILE:HD12	1.75	0.51
1:B:170:GLU:O	1:B:226:LYS:HG2	2.11	0.51
1:A:142:THR:HG22	1:A:143:MET:HG3	1.92	0.51
1:A:308:LYS:HB2	1:B:173:LEU:HD13	1.92	0.51
1:E:199:ARG:O	4:E:507:HOH:O	2.19	0.51
1:F:262:LYS:O	1:F:266:GLU:HG2	2.11	0.51
1:H:28:VAL:O	1:H:72:ILE:HD11	2.08	0.51
1:A:146:VAL:HG22	1:A:147:SER:N	2.26	0.51
1:E:185:LYS:NZ	4:E:514:HOH:O	2.43	0.51
1:E:146:VAL:HG22	1:E:147:SER:N	2.26	0.51
1:F:26:VAL:O	1:F:26:VAL:HG23	2.11	0.51
1:F:36:ILE:HG22	1:F:41:MET:HG3	1.92	0.51
1:E:23:HIS:CE1	1:E:325:ASP:OD1	2.63	0.51
1:G:138:TYR:HD1	1:G:143:MET:CE	2.24	0.51
1:G:31:VAL:HG11	1:G:41:MET:CE	2.42	0.50
1:E:204:ASN:ND2	1:F:283:SER:H	2.09	0.50
1:A:184:GLN:NE2	1:A:233:ARG:HH11	2.10	0.50
1:H:170:GLU:HG2	1:H:249:LYS:HG2	1.94	0.50
1:E:115:LYS:N	4:E:509:HOH:O	2.45	0.50
1:H:118:ILE:HD12	1:H:327:ILE:CG1	2.38	0.50
1:B:230:MET:C	4:B:505:HOH:O	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:HB3	1:B:142:THR:OG1	2.12	0.50
1:E:146:VAL:CG2	1:E:147:SER:N	2.75	0.50
1:A:173:LEU:HB3	1:B:308:LYS:HE2	1.93	0.50
1:C:195:TRP:HB2	1:D:279:GLN:HE21	1.77	0.50
1:A:28:VAL:O	1:A:72:ILE:HD11	2.10	0.49
1:E:184:GLN:NE2	1:E:233:ARG:HH11	2.09	0.49
1:A:101:THR:CG2	1:A:122:PRO:O	2.61	0.49
1:A:117:VAL:HG12	1:A:145:VAL:HA	1.94	0.49
1:A:196:ARG:HG3	1:B:279:GLN:HB3	1.94	0.49
1:C:170:GLU:HG2	1:C:249:LYS:HG2	1.95	0.49
1:D:138:TYR:HD1	1:D:143:MET:CE	2.26	0.49
1:A:210:THR:N	4:A:507:HOH:O	2.05	0.49
1:C:36:ILE:HG22	1:C:41:MET:HG3	1.94	0.49
1:F:23:HIS:HB2	1:F:26:VAL:HG22	1.95	0.49
1:B:79:ASP:HB3	4:B:503:HOH:O	2.11	0.49
1:D:184:GLN:NE2	1:D:233:ARG:HH11	2.10	0.49
1:B:166:ASN:N	1:B:166:ASN:HD22	2.10	0.49
1:A:146:VAL:CG2	1:A:147:SER:N	2.76	0.48
1:B:138:TYR:HA	1:B:143:MET:HE1	1.95	0.48
1:G:26:VAL:HG21	1:G:327:ILE:HD11	1.95	0.48
1:G:177:ILE:CD1	1:H:232:PHE:CD2	2.96	0.48
1:C:184:GLN:NE2	1:C:233:ARG:HH11	2.10	0.48
1:E:59:GLU:HB3	1:E:66:VAL:HG11	1.91	0.48
1:E:86:LYS:HB2	1:E:113:GLY:HA3	1.95	0.48
1:E:150:SER:O	1:E:153:THR:OG1	2.31	0.48
1:G:93:VAL:HG11	1:G:109:HIS:HB3	1.96	0.48
1:A:36:ILE:HG22	1:A:41:MET:HG3	1.95	0.48
1:E:245:THR:CB	4:E:505:HOH:O	2.45	0.48
1:D:17:MET:O	1:D:21:LEU:CD1	2.53	0.48
1:F:31:VAL:HG11	1:F:41:MET:HE3	1.95	0.48
1:A:86:LYS:HB2	1:A:113:GLY:HA3	1.95	0.48
1:D:170:GLU:OE1	1:D:249:LYS:HE3	2.14	0.48
1:F:138:TYR:HD1	1:F:143:MET:CE	2.25	0.48
1:A:180:TYR:HA	1:A:184:GLN:NE2	2.29	0.48
1:D:36:ILE:HD12	1:D:36:ILE:N	2.29	0.48
1:D:38:LEU:HD11	1:D:60:VAL:CG1	2.43	0.48
1:D:72:ILE:HD12	1:D:72:ILE:N	2.29	0.48
1:E:101:THR:CG2	1:E:122:PRO:O	2.62	0.48
1:E:246:CYS:N	4:E:505:HOH:O	2.47	0.48
1:G:6:ILE:CD1	1:G:94:VAL:HB	2.44	0.47
1:G:317:TYR:CE2	1:G:321:HIS:HE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:LYS:O	4:D:508:HOH:O	2.20	0.47
1:F:325:ASP:O	1:F:328:GLU:HG2	2.14	0.47
1:C:6:ILE:CD1	1:C:94:VAL:HB	2.44	0.47
1:A:59:GLU:HB3	1:A:66:VAL:HG11	1.92	0.47
1:B:330:MET:C	1:B:331:ALA:O	2.52	0.47
1:B:256:GLU:OE2	1:B:259:LYS:HD2	2.14	0.47
1:C:139:ASP:C	1:C:141:ALA:H	2.18	0.47
1:G:66:VAL:C	1:G:67:ILE:HD13	2.35	0.47
1:G:86:LYS:HB2	1:G:113:GLY:HA3	1.95	0.47
1:H:93:VAL:HG11	1:H:109:HIS:CD2	2.50	0.47
1:H:317:TYR:CE2	1:H:321:HIS:HE1	2.32	0.47
1:C:180:TYR:HA	1:C:184:GLN:NE2	2.30	0.47
1:C:204:ASN:ND2	1:D:283:SER:H	2.13	0.47
1:F:251:PRO:HG3	1:F:305:THR:CG2	2.45	0.47
1:G:31:VAL:HG11	1:G:41:MET:HE3	1.96	0.47
1:G:42:GLU:HG3	1:G:58:THR:OG1	2.14	0.47
1:D:110:LEU:C	1:D:112:GLY:O	2.53	0.46
1:G:36:ILE:HG22	1:G:41:MET:HG3	1.95	0.46
1:B:86:LYS:HB3	1:B:113:GLY:HA3	1.96	0.46
1:B:167:PHE:HE2	1:B:260:VAL:HG11	1.80	0.46
1:A:257:ILE:C	4:A:506:HOH:O	2.42	0.46
1:D:52:GLY:HA3	4:D:509:HOH:O	2.14	0.46
1:C:32:ASN:ND2	1:C:77:LEU:H	2.00	0.46
1:C:164:ASN:HB2	1:C:169:ILE:HD13	1.97	0.46
1:D:239:VAL:HG23	1:D:286:ILE:HD13	1.98	0.46
1:D:293:VAL:C	4:D:502:HOH:O	2.54	0.46
1:H:86:LYS:HB2	1:H:113:GLY:HA3	1.98	0.46
1:F:23:HIS:O	1:F:26:VAL:HG22	2.15	0.46
1:F:138:TYR:CD1	1:F:143:MET:HE2	2.51	0.46
1:B:79:ASP:C	4:B:503:HOH:O	2.54	0.46
1:E:180:TYR:HA	1:E:184:GLN:NE2	2.31	0.46
1:H:85:TRP:HE1	1:H:109:HIS:HD2	1.64	0.46
1:B:81:ALA:N	4:B:503:HOH:O	2.48	0.46
1:B:252:THR:OG1	1:B:253:SER:N	2.49	0.46
1:D:71:PRO:C	1:D:72:ILE:HD12	2.35	0.46
1:D:180:TYR:HA	1:D:184:GLN:NE2	2.31	0.46
1:D:258:LYS:NZ	4:D:515:HOH:O	2.44	0.46
1:E:68:ASN:CA	4:E:502:HOH:O	2.52	0.46
1:E:239:VAL:HG23	1:E:286:ILE:HD13	1.98	0.46
1:H:138:TYR:CD1	1:H:143:MET:HE2	2.50	0.46
1:A:219:VAL:HG23	1:A:220:ILE:CD1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:VAL:HG11	1:B:157:ALA:HB3	1.99	0.45
1:B:325:ASP:HA	1:B:328:GLU:OE1	2.16	0.45
1:C:31:VAL:CG1	1:C:41:MET:HE3	2.46	0.45
1:D:42:GLU:HG3	1:D:58:THR:OG1	2.16	0.45
1:G:25:GLU:H	1:G:25:GLU:CD	2.18	0.45
1:F:239:VAL:HG23	1:F:286:ILE:HD13	1.98	0.45
1:G:93:VAL:CG1	1:G:117:VAL:HG22	2.46	0.45
1:A:239:VAL:HG23	1:A:286:ILE:HD13	1.99	0.45
1:B:3:LYS:HB2	1:B:3:LYS:HE2	1.73	0.45
1:F:86:LYS:HB2	1:F:113:GLY:HA3	1.99	0.45
2:B:401:NAD:O1N	2:B:401:NAD:N7N	2.50	0.45
1:E:232:PHE:CD2	1:F:177:ILE:CD1	2.99	0.45
1:F:108:ALA:HA	1:F:111:HIS:CE1	2.52	0.45
1:G:138:TYR:CD1	1:G:143:MET:HE2	2.51	0.45
1:A:202:ASN:ND2	1:D:202:ASN:OD1	2.40	0.45
1:B:64:LYS:HD2	1:B:73:SER:HA	1.98	0.45
1:F:139:ASP:HB3	1:F:142:THR:CG2	2.46	0.45
1:A:117:VAL:CG1	1:A:145:VAL:HG13	2.47	0.45
1:A:303:ASN:HD21	1:B:171:GLU:CD	2.20	0.45
1:G:93:VAL:HG13	1:G:117:VAL:HG22	1.99	0.45
1:G:239:VAL:HG23	1:G:286:ILE:HD13	1.99	0.45
1:H:42:GLU:HG3	1:H:58:THR:OG1	2.17	0.44
1:D:138:TYR:CD1	1:D:143:MET:HE2	2.52	0.44
1:G:65:LEU:HG	1:G:67:ILE:CD1	2.48	0.44
1:B:11:ARG:HH11	1:B:14:ARG:NH2	2.15	0.44
1:C:112:GLY:HA3	4:C:504:HOH:O	2.17	0.44
1:D:157:ALA:HB3	1:D:158:PRO:HD3	2.00	0.44
1:E:155:CYS:C	4:E:504:HOH:O	2.30	0.44
1:B:42:GLU:O	1:B:46:LYS:HG3	2.17	0.44
1:C:157:ALA:HB3	1:C:158:PRO:HD3	2.00	0.44
1:D:53:ARG:N	4:D:509:HOH:O	2.21	0.44
1:E:129:PHE:HD2	1:E:146:VAL:HG23	1.76	0.44
1:F:193:LYS:N	1:F:193:LYS:HD3	2.32	0.44
1:A:230:MET:CE	1:B:308:LYS:HD2	2.48	0.44
1:B:23:HIS:HB3	1:B:25:GLU:CD	2.38	0.44
1:D:27:GLN:HE21	1:D:27:GLN:HB3	1.58	0.44
1:F:252:THR:OG1	1:F:253:SER:N	2.47	0.44
1:A:230:MET:HE1	1:B:298:ALA:O	2.17	0.44
1:B:36:ILE:HG22	1:B:41:MET:HG3	1.99	0.44
1:C:163:ILE:HG22	1:C:169:ILE:HD11	1.99	0.44
1:H:239:VAL:HG23	1:H:286:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:MET:HE1	1:C:215:ALA:CB	2.48	0.43
1:C:239:VAL:HG23	1:C:286:ILE:HD13	1.98	0.43
1:F:251:PRO:HG3	1:F:305:THR:HG22	1.99	0.43
1:A:209:THR:CA	4:A:507:HOH:O	2.65	0.43
2:A:401:NAD:O1A	4:A:510:HOH:O	2.21	0.43
1:B:64:LYS:HE3	1:B:73:SER:HB3	2.00	0.43
1:C:332:THR:O	1:C:333:LYS:C	2.56	0.43
1:D:85:TRP:HE1	1:D:109:HIS:HD2	1.65	0.43
1:C:333:LYS:N	1:C:333:LYS:HD3	2.33	0.43
1:H:87:GLU:O	1:H:88:ALA:CB	2.56	0.43
1:C:328:GLU:O	1:C:332:THR:HG23	2.17	0.43
1:E:45:PHE:O	4:E:508:HOH:O	2.21	0.43
1:E:118:ILE:HD13	1:E:146:VAL:CG1	2.49	0.43
1:F:194:LYS:HG3	1:F:197:ASP:CG	2.39	0.43
1:E:245:THR:OG1	1:F:245:THR:HG21	2.19	0.43
1:F:23:HIS:HB2	1:F:26:VAL:CG2	2.48	0.43
1:G:157:ALA:HB3	1:G:158:PRO:HD3	2.01	0.43
1:A:243:ASP:OD2	1:B:175:THR:OG1	2.19	0.43
1:C:86:LYS:HB2	1:C:113:GLY:HA3	2.00	0.43
1:C:138:TYR:HD1	1:C:143:MET:HE3	1.81	0.43
1:E:28:VAL:O	1:E:28:VAL:CG2	2.66	0.43
1:B:210:THR:CG2	4:B:505:HOH:O	2.49	0.43
1:A:232:PHE:CD2	1:B:177:ILE:HD12	2.54	0.43
1:F:157:ALA:HB3	1:F:158:PRO:HD3	2.01	0.43
1:H:27:GLN:HG3	1:H:70:ASN:ND2	2.34	0.43
1:A:6:ILE:HB	1:A:31:VAL:HG12	2.01	0.42
1:A:157:ALA:HB3	1:A:158:PRO:HD3	2.01	0.42
1:D:118:ILE:HD13	1:D:146:VAL:CG2	2.48	0.42
1:G:61:LYS:CD	1:G:62:ASP:OD2	2.67	0.42
1:H:27:GLN:CG	1:H:70:ASN:HD21	2.32	0.42
1:H:157:ALA:HB3	1:H:158:PRO:HD3	2.01	0.42
1:B:139:ASP:H	1:B:143:MET:CE	2.31	0.42
1:B:254:TYR:N	1:B:301:GLN:OE1	2.53	0.42
1:A:129:PHE:CE2	1:A:146:VAL:HG23	2.54	0.42
1:B:23:HIS:HE1	1:B:321:HIS:ND1	2.16	0.42
1:E:220:ILE:HG22	1:E:222:GLU:HG2	2.00	0.42
1:B:103:THR:HG23	1:B:145:VAL:CG2	2.50	0.42
1:B:107:SER:HA	1:B:110:LEU:HD23	2.02	0.42
1:B:118:ILE:HD12	1:B:327:ILE:HG12	2.02	0.42
1:C:6:ILE:HD12	1:C:94:VAL:HB	2.01	0.42
1:C:128:MET:HE1	1:C:215:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:PHE:HB2	1:D:36:ILE:HD12	2.01	0.42
1:E:170:GLU:HG3	1:E:249:LYS:HG2	2.00	0.42
1:H:85:TRP:HE1	1:H:109:HIS:CD2	2.38	0.42
1:E:204:ASN:HD22	1:F:283:SER:H	1.65	0.42
1:C:11:ARG:O	1:C:15:LEU:HD22	2.19	0.42
1:C:138:TYR:C	1:C:143:MET:HE1	2.36	0.42
1:D:170:GLU:HG2	1:D:247:ARG:NH2	2.34	0.42
1:E:173:LEU:HD13	1:F:308:LYS:HB2	2.01	0.42
1:G:23:HIS:CD2	1:G:328:GLU:OE2	2.72	0.42
1:B:230:MET:CA	4:B:505:HOH:O	2.67	0.42
1:E:170:GLU:OE1	1:E:247:ARG:HG2	2.20	0.42
1:C:11:ARG:O	1:C:15:LEU:CD2	2.67	0.42
1:E:115:LYS:HG2	4:E:509:HOH:O	2.20	0.42
1:E:153:THR:HG21	1:E:215:ALA:HB3	2.02	0.42
1:B:86:LYS:H	1:B:86:LYS:HG2	1.64	0.41
1:E:17:MET:CE	1:E:72:ILE:HD13	2.50	0.41
1:E:157:ALA:HB3	1:E:158:PRO:HD3	2.02	0.41
1:F:10:GLY:O	1:F:14:ARG:HG3	2.20	0.41
1:D:10:GLY:HA3	2:D:401:NAD:O5B	2.20	0.41
1:D:303:ASN:HB2	1:D:304:PRO:CD	2.51	0.41
1:H:303:ASN:HB2	1:H:304:PRO:CD	2.51	0.41
1:D:103:THR:HG22	1:D:126:ALA:HB2	2.02	0.41
1:E:219:VAL:HG23	1:E:220:ILE:CD1	2.27	0.41
1:F:167:PHE:CD1	1:F:252:THR:CG2	3.03	0.41
2:G:401:NAD:H3B	4:G:516:HOH:O	2.19	0.41
1:B:139:ASP:H	1:B:143:MET:HE2	1.86	0.41
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.71	0.41
1:D:85:TRP:HE1	1:D:109:HIS:CD2	2.38	0.41
1:E:170:GLU:HG3	1:E:249:LYS:CD	2.50	0.41
1:A:194:LYS:N	4:A:503:HOH:O	2.45	0.41
1:A:256:GLU:O	4:A:506:HOH:O	2.22	0.41
1:A:258:LYS:HE2	4:A:508:HOH:O	2.20	0.41
1:D:301:GLN:HE21	1:D:304:PRO:HA	1.86	0.41
1:E:52:GLY:HA2	4:G:517:HOH:O	2.21	0.41
1:A:301:GLN:HE21	1:A:304:PRO:HA	1.86	0.41
1:B:31:VAL:O	1:B:74:VAL:HA	2.21	0.41
1:B:127:PRO:HG2	1:B:146:VAL:HG12	2.03	0.41
1:C:301:GLN:HE21	1:C:304:PRO:HA	1.86	0.41
1:C:303:ASN:HB2	1:C:304:PRO:CD	2.51	0.41
1:E:170:GLU:HG3	1:E:249:LYS:HE3	2.03	0.41
1:E:303:ASN:HB2	1:E:304:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ARG:HA	1:B:11:ARG:HD2	1.92	0.41
1:E:118:ILE:CD1	1:E:330:MET:SD	3.09	0.41
1:G:303:ASN:HB2	1:G:304:PRO:CD	2.51	0.41
1:B:26:VAL:HG21	1:B:324:VAL:CG1	2.51	0.40
1:B:167:PHE:HB2	1:B:248:LEU:HD23	2.03	0.40
1:E:279:GLN:NE2	1:F:195:TRP:HB2	2.35	0.40
1:F:301:GLN:HE21	1:F:304:PRO:HA	1.86	0.40
1:A:77:LEU:N	1:A:77:LEU:CD1	2.84	0.40
1:D:328:GLU:O	1:D:332:THR:HG23	2.21	0.40
1:A:303:ASN:HB2	1:A:304:PRO:CD	2.51	0.40
1:B:107:SER:HA	1:B:110:LEU:CD2	2.51	0.40
1:F:303:ASN:HB2	1:F:304:PRO:CD	2.51	0.40
1:F:328:GLU:O	1:F:332:THR:HG23	2.21	0.40
1:A:232:PHE:CD2	1:B:177:ILE:CD1	3.04	0.40
1:B:248:LEU:HD11	1:B:307:VAL:HG12	2.03	0.40
1:G:139:ASP:HB3	1:G:142:THR:CG2	2.46	0.40
1:H:27:GLN:HG3	1:H:70:ASN:HD21	1.85	0.40
1:B:36:ILE:CG2	1:B:41:MET:HG3	2.51	0.40
1:C:23:HIS:CD2	1:C:328:GLU:OE2	2.75	0.40
1:C:139:ASP:OD2	1:C:141:ALA:HB3	2.22	0.40
1:D:17:MET:HG2	1:D:45:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/355 (93%)	312 (94%)	15 (4%)	3 (1%)	17	25
1	B	330/355 (93%)	308 (93%)	18 (6%)	4 (1%)	13	19
1	C	330/355 (93%)	309 (94%)	20 (6%)	1 (0%)	41	55
1	D	330/355 (93%)	313 (95%)	16 (5%)	1 (0%)	41	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	330/355 (93%)	314 (95%)	14 (4%)	2 (1%)	25	36
1	F	330/355 (93%)	310 (94%)	19 (6%)	1 (0%)	41	55
1	G	330/355 (93%)	314 (95%)	14 (4%)	2 (1%)	25	36
1	H	330/355 (93%)	313 (95%)	16 (5%)	1 (0%)	41	55
All	All	2640/2840 (93%)	2493 (94%)	132 (5%)	15 (1%)	25	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	B	331	ALA
1	A	141	ALA
1	A	239	VAL
1	B	168	GLY
1	B	224	ASN
1	B	239	VAL
1	C	239	VAL
1	D	239	VAL
1	E	239	VAL
1	E	332	THR
1	F	239	VAL
1	G	141	ALA
1	G	239	VAL
1	H	239	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/297 (93%)	269 (98%)	6 (2%)	52	71
1	B	274/297 (92%)	265 (97%)	9 (3%)	38	57
1	C	275/297 (93%)	271 (98%)	4 (2%)	65	80
1	D	275/297 (93%)	267 (97%)	8 (3%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	275/297 (93%)	270 (98%)	5 (2%)	59 76
1	F	275/297 (93%)	273 (99%)	2 (1%)	84 92
1	G	275/297 (93%)	271 (98%)	4 (2%)	65 80
1	H	275/297 (93%)	271 (98%)	4 (2%)	65 80
All	All	2199/2376 (93%)	2157 (98%)	42 (2%)	57 75

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	77	LEU
1	A	86	LYS
1	A	142	THR
1	A	193	LYS
1	A	328	GLU
1	B	3	LYS
1	B	9	PHE
1	B	111	HIS
1	B	226	LYS
1	B	246	CYS
1	B	259	LYS
1	B	265	SER
1	B	313	TYR
1	B	317	TYR
1	C	87	GLU
1	C	142	THR
1	C	143	MET
1	C	333	LYS
1	D	21	LEU
1	D	27	GLN
1	D	38	LEU
1	D	77	LEU
1	D	115	LYS
1	D	142	THR
1	D	170	GLU
1	D	256	GLU
1	E	115	LYS
1	E	136	LYS
1	E	175	THR
1	E	256	GLU
1	E	333	LYS

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Mol	Chain	Res	Type
1	F	259	LYS
1	F	266	GLU
1	G	50	THR
1	G	61	LYS
1	G	67	ILE
1	G	115	LYS
1	H	38	LEU
1	H	77	LEU
1	H	86	LYS
1	H	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	184	GLN
1	A	202	ASN
1	A	224	ASN
1	B	27	GLN
1	B	166	ASN
1	C	32	ASN
1	C	184	GLN
1	C	204	ASN
1	C	290	HIS
1	D	27	GLN
1	D	109	HIS
1	D	184	GLN
1	D	279	GLN
1	E	70	ASN
1	E	184	GLN
1	E	204	ASN
1	E	279	GLN
1	F	23	HIS
1	F	290	HIS
1	G	23	HIS
1	G	70	ASN
1	G	148	ASN
1	G	279	GLN
1	G	321	HIS
1	H	109	HIS
1	H	321	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 monosaccharides in this entry.

5.6 Ligand geometry

16 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	C	401	-	42,48,48	0.91	3 (7%)	50,73,73	1.25	6 (12%)
3	PO4	A	402	-	4,4,4	0.92	0	6,6,6	0.90	0
2	NAD	H	401	-	42,48,48	0.95	4 (9%)	50,73,73	1.26	6 (12%)
2	NAD	E	401	-	42,48,48	0.89	2 (4%)	50,73,73	1.32	7 (14%)
2	NAD	A	401	-	42,48,48	0.84	1 (2%)	50,73,73	1.21	4 (8%)
3	PO4	B	402	-	4,4,4	0.77	0	6,6,6	0.41	0
3	PO4	C	402	-	4,4,4	0.97	0	6,6,6	0.79	0
3	PO4	G	402	-	4,4,4	0.90	0	6,6,6	0.67	0
3	PO4	D	402	-	4,4,4	0.91	0	6,6,6	0.79	0
2	NAD	G	401	-	42,48,48	0.93	3 (7%)	50,73,73	1.18	5 (10%)
2	NAD	F	401	-	42,48,48	0.84	3 (7%)	50,73,73	1.24	5 (10%)
3	PO4	F	402	-	4,4,4	0.96	0	6,6,6	0.60	0
2	NAD	D	401	-	42,48,48	0.91	4 (9%)	50,73,73	1.21	4 (8%)
3	PO4	E	402	-	4,4,4	0.96	0	6,6,6	0.66	0
2	NAD	B	401	-	42,48,48	0.68	1 (2%)	50,73,73	0.78	2 (4%)
3	PO4	H	402	-	4,4,4	0.84	0	6,6,6	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	401	-	-	7/26/62/62	0/5/5/5
2	NAD	H	401	-	-	5/26/62/62	0/5/5/5
2	NAD	E	401	-	-	3/26/62/62	0/5/5/5
2	NAD	A	401	-	-	7/26/62/62	0/5/5/5
2	NAD	G	401	-	-	8/26/62/62	0/5/5/5
2	NAD	F	401	-	-	9/26/62/62	0/5/5/5
2	NAD	D	401	-	-	4/26/62/62	0/5/5/5
2	NAD	B	401	-	-	9/26/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	NAD	C5A-C4A	2.81	1.48	1.40
2	C	401	NAD	C5A-C4A	2.63	1.47	1.40
2	A	401	NAD	C5A-C4A	2.48	1.47	1.40
2	E	401	NAD	C5A-C4A	2.47	1.47	1.40
2	F	401	NAD	C5A-C4A	2.46	1.47	1.40
2	G	401	NAD	C2A-N3A	2.44	1.36	1.32
2	H	401	NAD	O4D-C1D	2.44	1.44	1.41
2	D	401	NAD	C5A-C4A	2.43	1.47	1.40
2	D	401	NAD	O4D-C1D	2.40	1.44	1.41
2	H	401	NAD	C5A-C4A	2.40	1.47	1.40
2	G	401	NAD	O4D-C1D	2.35	1.44	1.41
2	H	401	NAD	O4B-C1B	2.29	1.44	1.41
2	B	401	NAD	C2N-N1N	2.28	1.37	1.35
2	C	401	NAD	C2A-N3A	2.27	1.35	1.32
2	E	401	NAD	O4D-C1D	2.24	1.44	1.41
2	C	401	NAD	O4D-C1D	2.19	1.44	1.41
2	F	401	NAD	C2A-N3A	2.15	1.35	1.32
2	H	401	NAD	C2A-N3A	2.07	1.35	1.32
2	D	401	NAD	O4B-C1B	2.06	1.43	1.41
2	F	401	NAD	O4D-C1D	2.05	1.43	1.41
2	D	401	NAD	C2A-N3A	2.02	1.35	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	401	NAD	N3A-C2A-N1A	-4.11	122.25	128.68
2	D	401	NAD	N3A-C2A-N1A	-3.96	122.48	128.68
2	F	401	NAD	N3A-C2A-N1A	-3.84	122.67	128.68
2	E	401	NAD	N3A-C2A-N1A	-3.69	122.91	128.68
2	A	401	NAD	N3A-C2A-N1A	-3.50	123.20	128.68
2	C	401	NAD	N3A-C2A-N1A	-3.50	123.20	128.68
2	D	401	NAD	C4A-C5A-N7A	-3.33	105.93	109.40
2	G	401	NAD	N3A-C2A-N1A	-3.30	123.53	128.68
2	D	401	NAD	PN-O3-PA	-3.25	121.67	132.83
2	C	401	NAD	C4A-C5A-N7A	-3.23	106.03	109.40
2	E	401	NAD	C4A-C5A-N7A	-3.13	106.13	109.40
2	G	401	NAD	C4A-C5A-N7A	-3.12	106.15	109.40
2	A	401	NAD	C4A-C5A-N7A	-2.99	106.29	109.40
2	F	401	NAD	PN-O3-PA	-2.86	123.00	132.83
2	A	401	NAD	PN-O3-PA	-2.82	123.15	132.83
2	E	401	NAD	C3N-C7N-N7N	2.74	121.03	117.75
2	H	401	NAD	C4A-C5A-N7A	-2.67	106.62	109.40
2	F	401	NAD	C4A-C5A-N7A	-2.66	106.63	109.40
2	B	401	NAD	C6N-N1N-C2N	-2.58	119.62	121.97
2	E	401	NAD	PN-O3-PA	-2.55	124.06	132.83
2	H	401	NAD	PN-O3-PA	-2.51	124.22	132.83
2	C	401	NAD	PN-O3-PA	-2.47	124.36	132.83
2	F	401	NAD	C3B-C2B-C1B	2.46	104.68	100.98
2	F	401	NAD	C3D-C2D-C1D	2.42	104.62	100.98
2	G	401	NAD	PN-O3-PA	-2.41	124.55	132.83
2	E	401	NAD	C2A-N1A-C6A	2.26	122.62	118.75
2	C	401	NAD	C3N-C7N-N7N	2.22	120.41	117.75
2	C	401	NAD	O2N-PN-O1N	2.21	123.14	112.24
2	E	401	NAD	O2A-PA-O1A	2.18	123.02	112.24
2	E	401	NAD	C1B-N9A-C4A	-2.16	122.84	126.64
2	B	401	NAD	C5A-C6A-N6A	2.14	123.60	120.35
2	A	401	NAD	O7N-C7N-C3N	-2.12	117.09	119.63
2	D	401	NAD	C1B-N9A-C4A	-2.11	122.94	126.64
2	H	401	NAD	C2A-N1A-C6A	2.09	122.33	118.75
2	H	401	NAD	C1B-N9A-C4A	-2.08	122.99	126.64
2	H	401	NAD	C6N-N1N-C2N	-2.07	120.08	121.97
2	G	401	NAD	C3B-C2B-C1B	2.04	104.05	100.98
2	C	401	NAD	C2A-N1A-C6A	2.03	122.22	118.75
2	G	401	NAD	O2N-PN-O1N	2.01	122.15	112.24

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C5B-O5B-PA-O1A
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C2N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C5B-O5B-PA-O1A
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	H	401	NAD	O4D-C1D-N1N-C2N
2	H	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	D	401	NAD	C3B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	C5B-O5B-PA-O3
2	F	401	NAD	C5B-O5B-PA-O3
2	G	401	NAD	PN-O3-PA-O1A
2	A	401	NAD	C4N-C3N-C7N-N7N
2	C	401	NAD	C4N-C3N-C7N-N7N
2	A	401	NAD	C4N-C3N-C7N-O7N
2	F	401	NAD	PN-O3-PA-O1A
2	C	401	NAD	C4N-C3N-C7N-O7N
2	C	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	G	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	G	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	PN-O3-PA-O2A
2	G	401	NAD	PN-O3-PA-O2A
2	G	401	NAD	C4N-C3N-C7N-O7N
2	B	401	NAD	C5B-O5B-PA-O2A
2	E	401	NAD	O4B-C4B-C5B-O5B
2	H	401	NAD	O4B-C4B-C5B-O5B
2	H	401	NAD	C4N-C3N-C7N-N7N
2	G	401	NAD	C4N-C3N-C7N-N7N

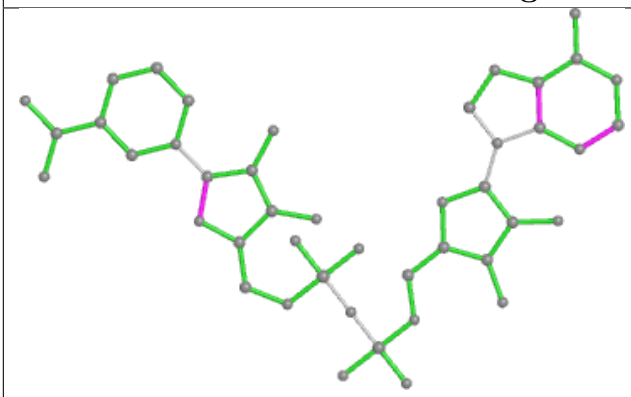
There are no ring outliers.

6 monomers are involved in 15 short contacts:

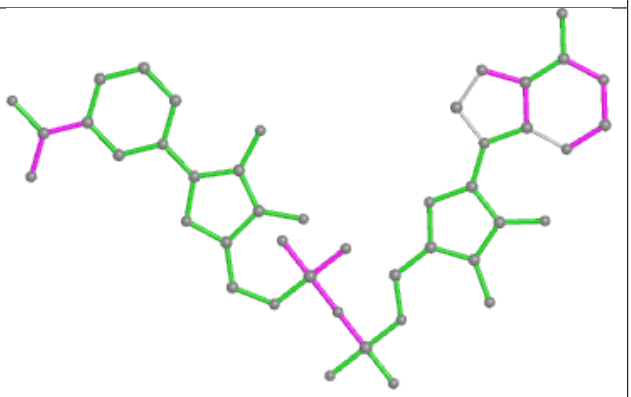
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	NAD	1	0
2	E	401	NAD	2	0
2	A	401	NAD	2	0
2	G	401	NAD	2	0
2	D	401	NAD	5	0
2	B	401	NAD	3	0

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 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 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.

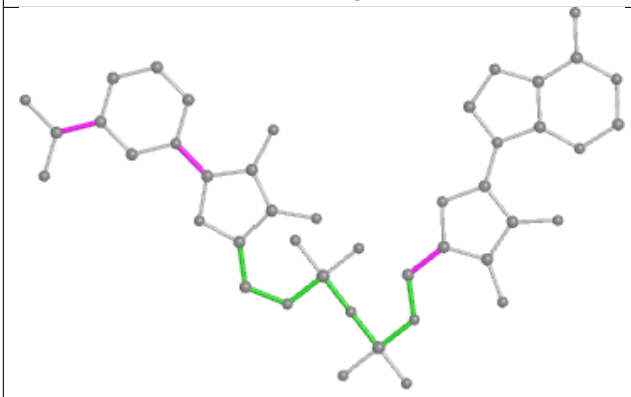
Ligand NAD C 401



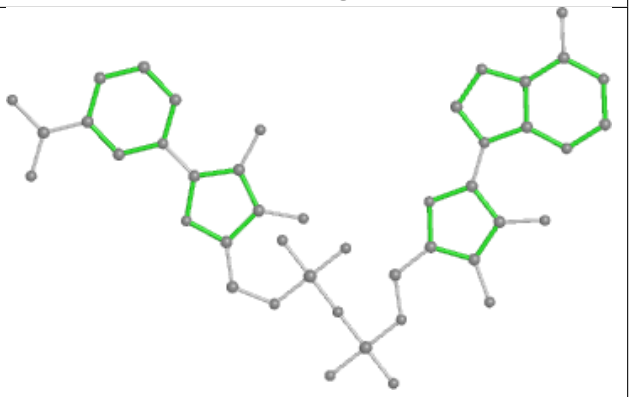
Bond lengths



Bond angles

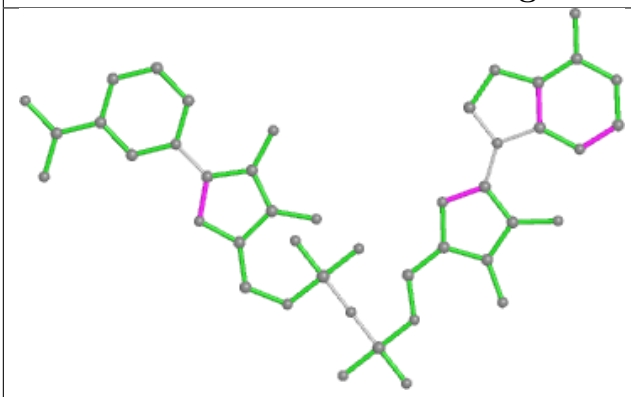


Torsions



Rings

Ligand NAD H 401



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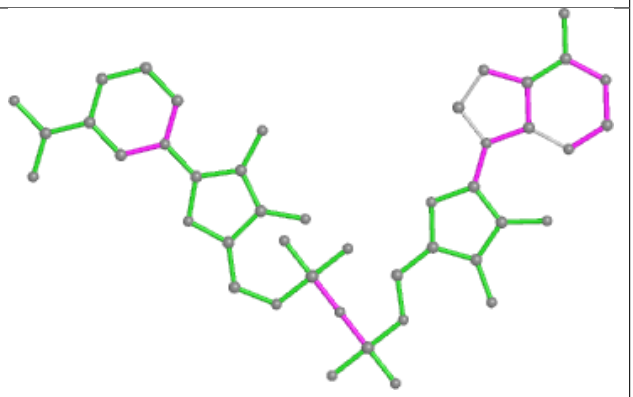
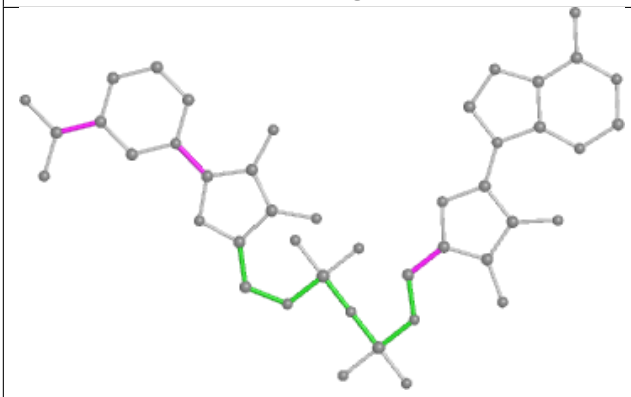


Bond angles



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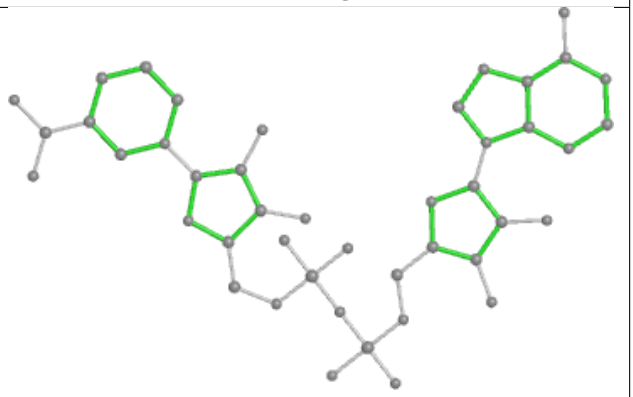
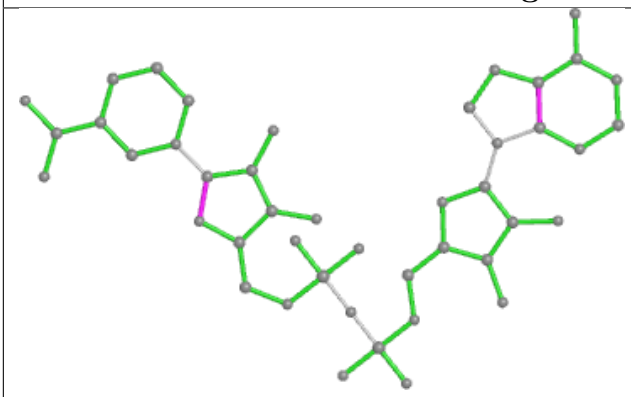
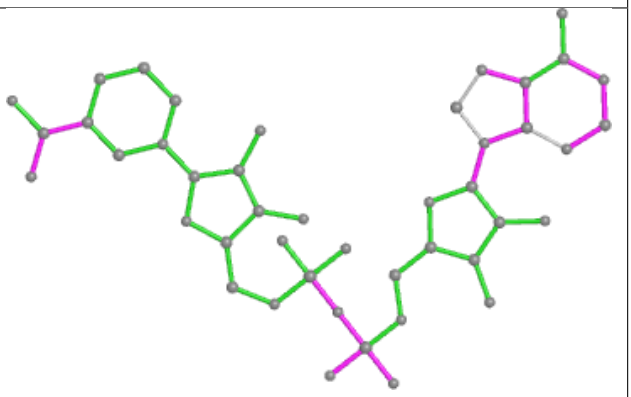


Rings

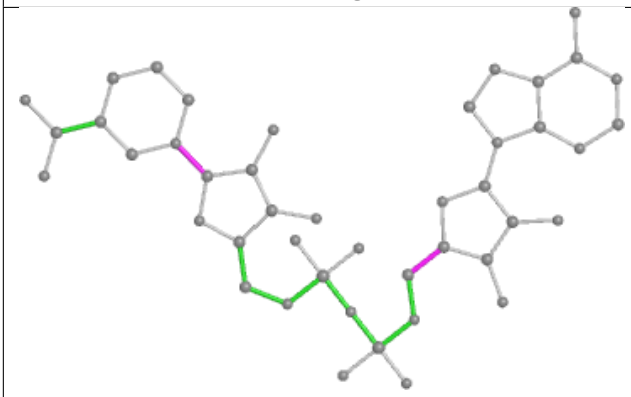
Ligand NAD E 401



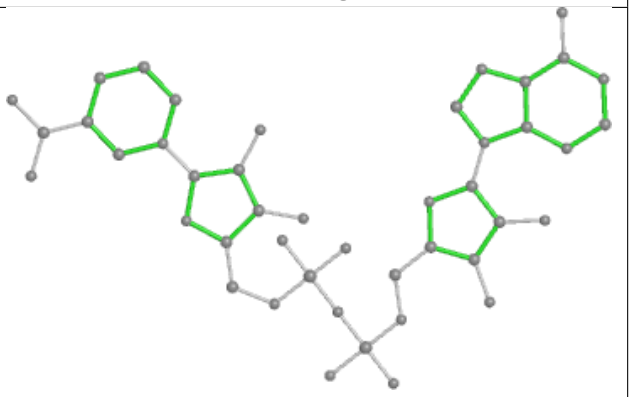
Bond lengths



Bond angles

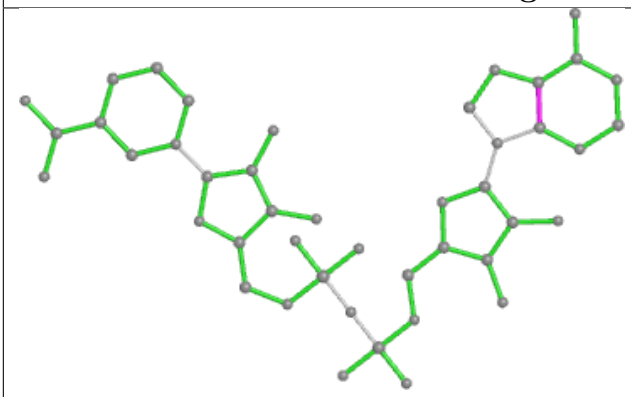


Torsions

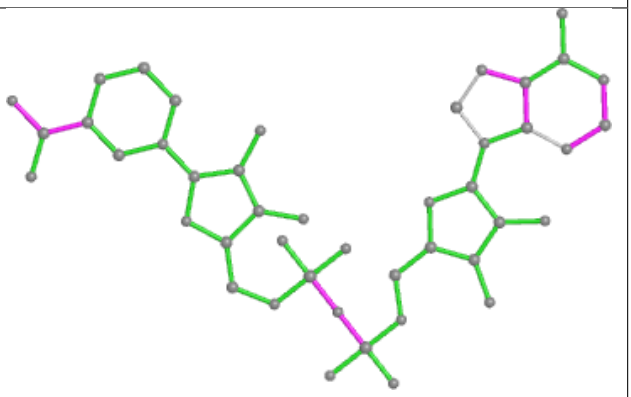


Rings

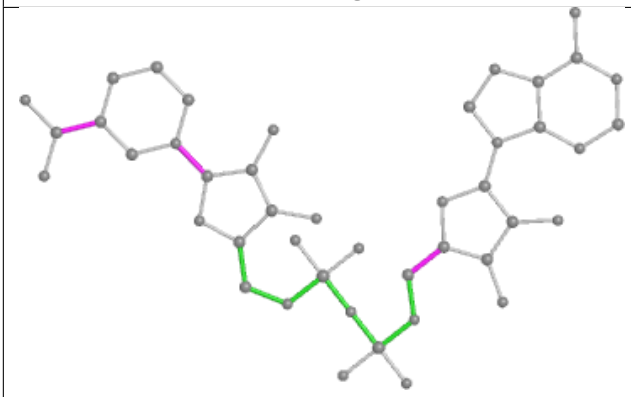
Ligand NAD A 401



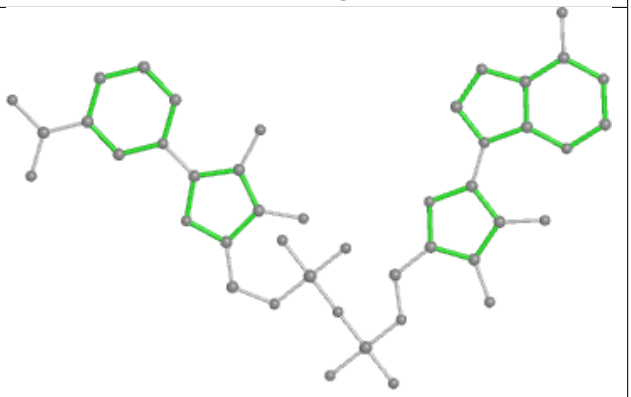
Bond lengths



Bond angles

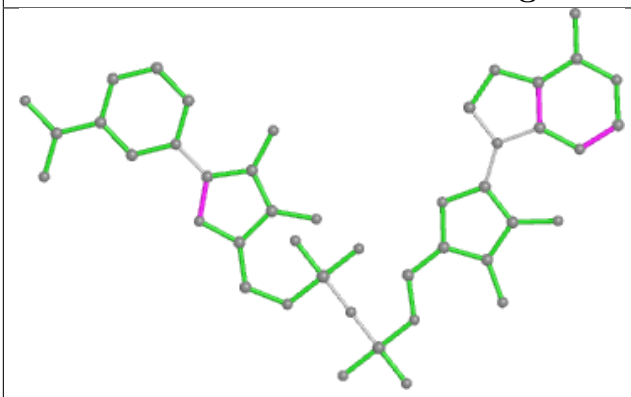


Torsions

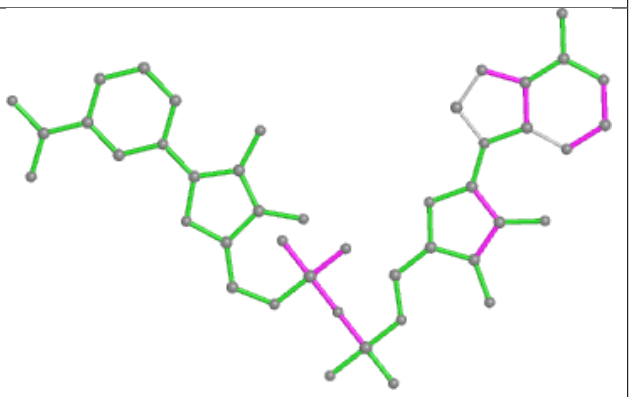


Rings

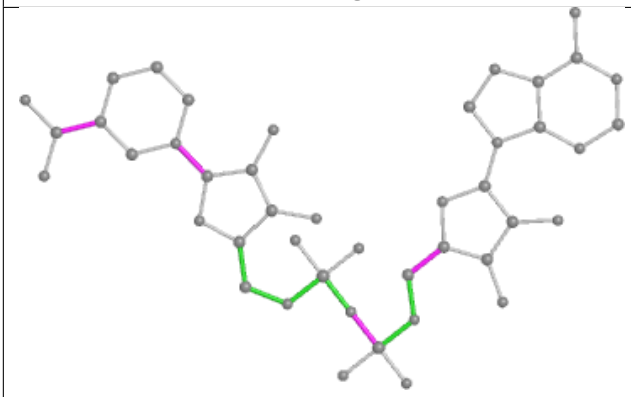
Ligand NAD G 401



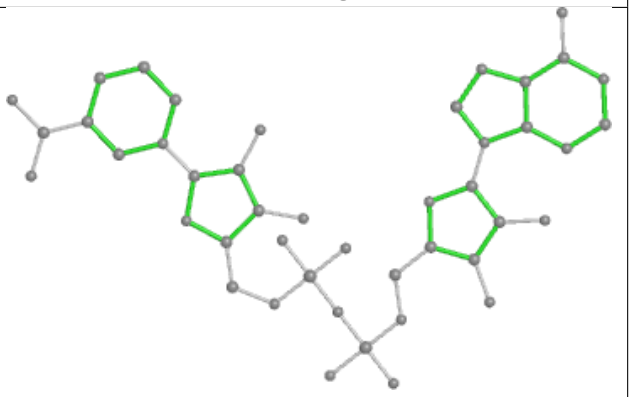
Bond lengths



Bond angles

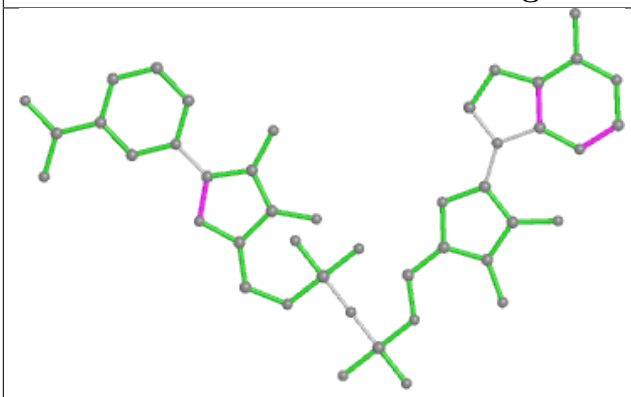


Torsions

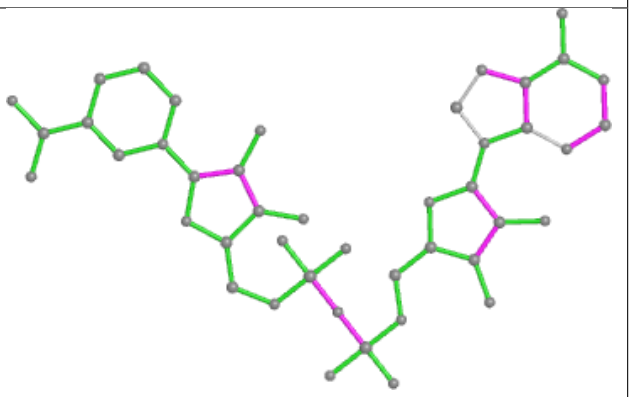


Rings

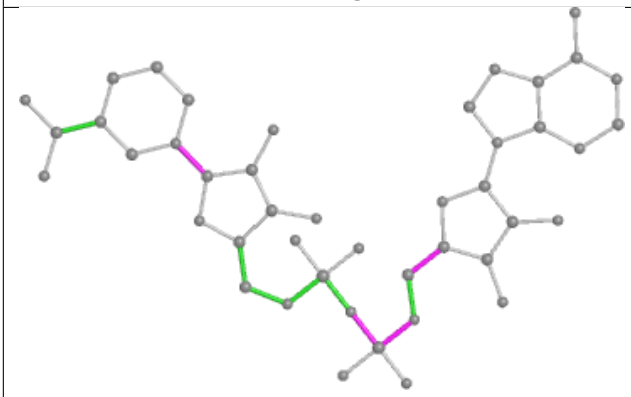
Ligand NAD F 401



Bond lengths



Bond angles



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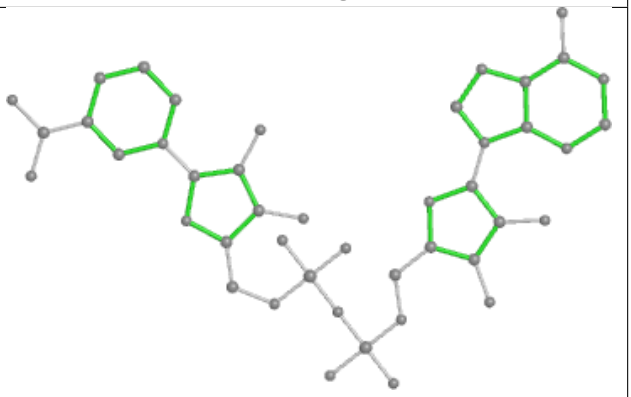
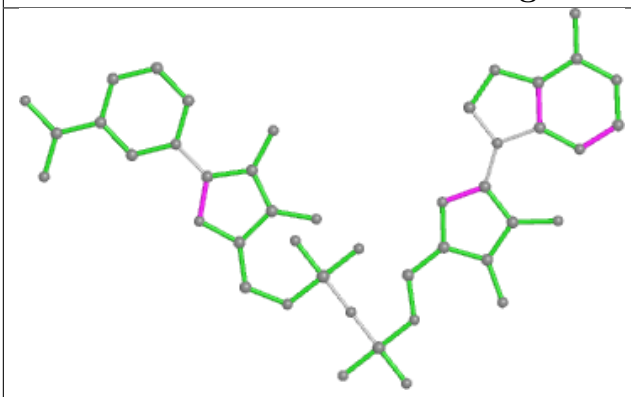
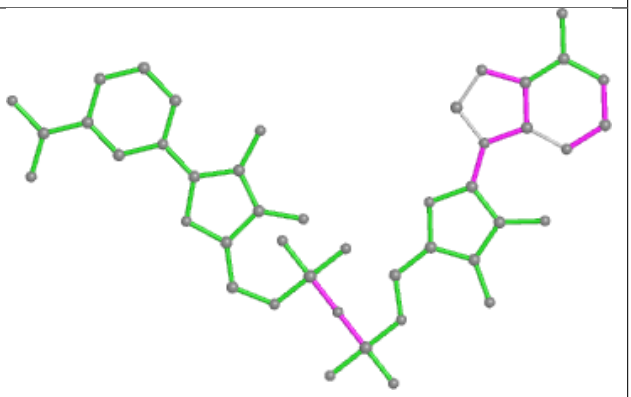


Rings

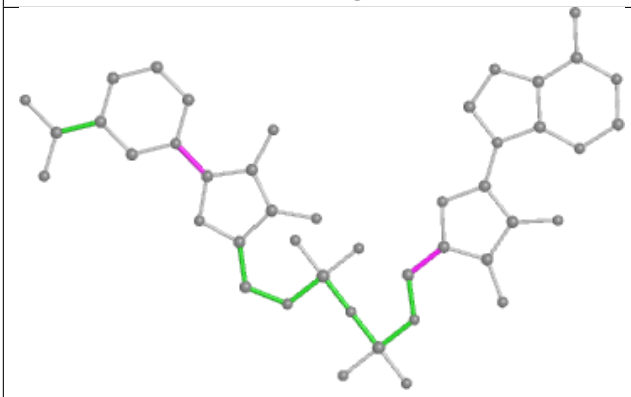
Ligand NAD D 401



Bond lengths



Bond angles



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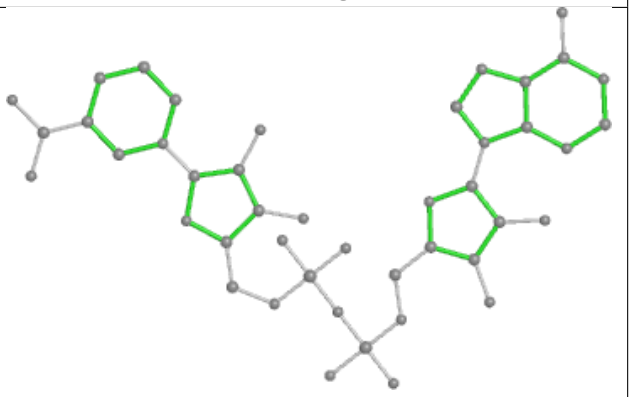
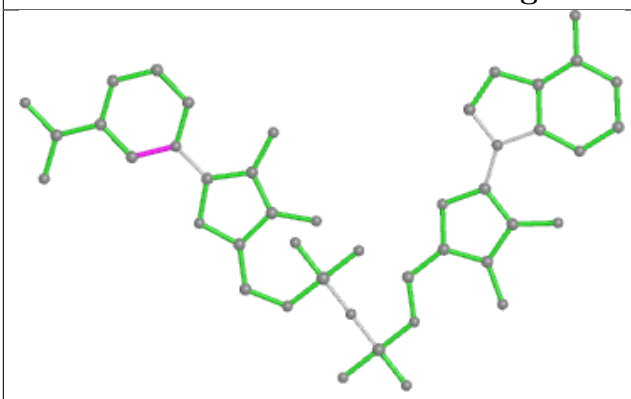
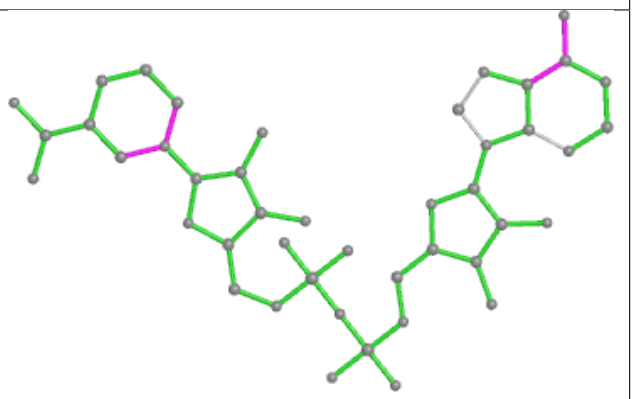


Rings

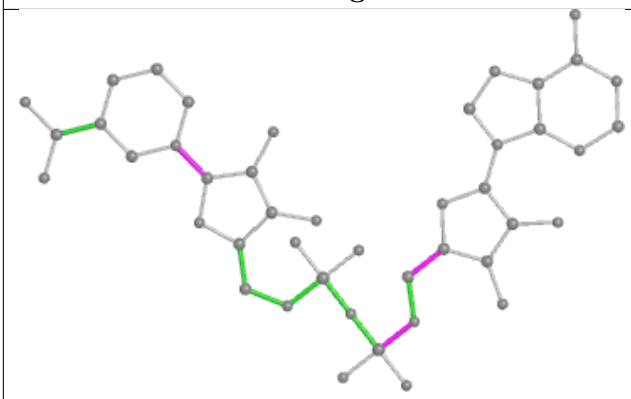
Ligand NAD B 401



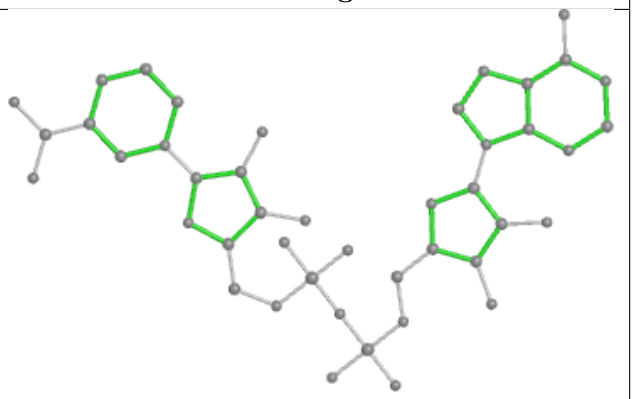
Bond lengths



Bond angles



Torsions



Rings

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^{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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	332/355 (93%)	-0.10	11 (3%)	46	45	37, 72, 104, 127	0
1	B	332/355 (93%)	0.04	17 (5%)	28	26	34, 72, 110, 130	0
1	C	332/355 (93%)	-0.10	17 (5%)	28	26	33, 66, 103, 124	0
1	D	332/355 (93%)	-0.22	9 (2%)	54	52	33, 61, 93, 115	0
1	E	332/355 (93%)	-0.14	8 (2%)	59	57	34, 67, 102, 132	0
1	F	332/355 (93%)	-0.03	12 (3%)	42	42	31, 69, 113, 137	0
1	G	332/355 (93%)	-0.16	12 (3%)	42	42	29, 64, 99, 128	0
1	H	332/355 (93%)	-0.31	5 (1%)	73	72	26, 58, 86, 106	0
All	All	2656/2840 (93%)	-0.13	91 (3%)	45	44	26, 66, 104, 137	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	251	PRO	4.8
1	C	141	ALA	4.7
1	G	141	ALA	4.7
1	G	93	VAL	4.1
1	G	24	PRO	4.0
1	E	332	THR	4.0
1	G	118	ILE	3.7
1	C	93	VAL	3.7
1	D	118	ILE	3.6
1	F	268	ASP	3.4
1	B	222	GLU	3.2
1	G	55	LYS	3.2
1	B	141	ALA	3.1
1	C	118	ILE	3.1
1	B	159	LEU	3.1
1	F	170	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	193	LYS	3.0
1	E	93	VAL	3.0
1	A	69	GLY	3.0
1	B	102	THR	2.9
1	B	142	THR	2.9
1	B	268	ASP	2.9
1	E	136	LYS	2.9
1	B	113	GLY	2.9
1	G	6	ILE	2.8
1	A	249	LYS	2.8
1	G	69	GLY	2.8
1	F	333	LYS	2.8
1	B	87	GLU	2.7
1	E	246	CYS	2.7
1	B	115	LYS	2.7
1	D	99	VAL	2.7
1	C	25	GLU	2.7
1	F	159	LEU	2.6
1	C	104	GLU	2.6
1	C	268	ASP	2.6
1	H	193	LYS	2.6
1	A	142	THR	2.6
1	B	333	LYS	2.6
1	A	246	CYS	2.5
1	G	35	PHE	2.5
1	C	142	THR	2.5
1	A	136	LYS	2.5
1	G	117	VAL	2.5
1	B	251	PRO	2.4
1	H	118	ILE	2.4
1	A	88	ALA	2.4
1	G	159	LEU	2.4
1	E	86	LYS	2.4
1	A	118	ILE	2.4
1	B	329	TYR	2.3
1	C	246	CYS	2.3
1	G	249	LYS	2.3
1	D	89	GLY	2.3
1	F	118	ILE	2.3
1	C	331	ALA	2.3
1	E	244	LEU	2.3
1	F	86	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	333	LYS	2.2
1	F	217	GLY	2.2
1	D	93	VAL	2.2
1	C	266	GLU	2.2
1	A	141	ALA	2.2
1	D	159	LEU	2.2
1	C	94	VAL	2.2
1	C	146	VAL	2.2
1	H	246	CYS	2.2
1	D	249	LYS	2.2
1	F	193	LYS	2.2
1	F	247	ARG	2.2
1	C	99	VAL	2.2
1	B	193	LYS	2.2
1	C	139	ASP	2.2
1	A	193	LYS	2.2
1	H	94	VAL	2.2
1	D	62	ASP	2.2
1	D	163	ILE	2.2
1	F	62	ASP	2.2
1	H	89	GLY	2.2
1	B	90	ALA	2.1
1	B	91	ASP	2.1
1	G	266	GLU	2.1
1	B	55	LYS	2.1
1	C	55	LYS	2.1
1	A	124	ALA	2.0
1	C	117	VAL	2.0
1	E	263	LYS	2.0
1	F	252	THR	2.0
1	B	86	LYS	2.0
1	E	159	LEU	2.0
1	A	86	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

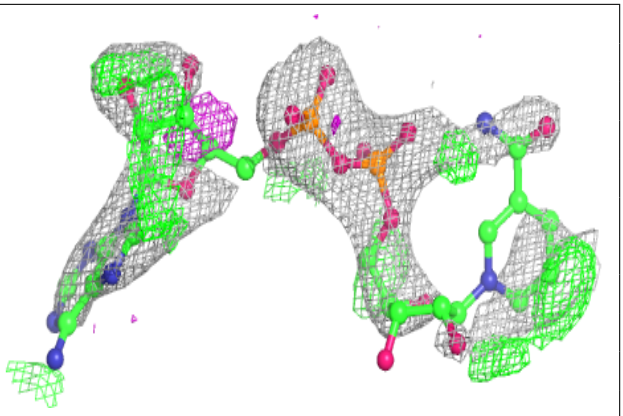
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

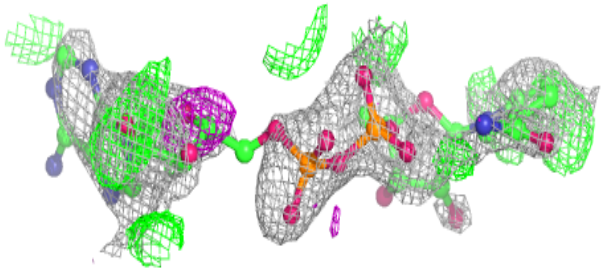
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	F	401	44/44	0.67	0.36	50,69,92,98	44
2	NAD	B	401	44/44	0.72	0.29	65,88,97,98	44
2	NAD	D	401	44/44	0.87	0.15	47,70,79,84	44
2	NAD	G	401	44/44	0.87	0.17	38,64,73,75	44
2	NAD	H	401	44/44	0.89	0.15	42,58,71,78	44
3	PO4	A	402	5/5	0.90	0.16	55,58,77,82	0
2	NAD	C	401	44/44	0.91	0.16	45,65,82,85	44
2	NAD	A	401	44/44	0.94	0.13	37,65,109,119	0
3	PO4	E	402	5/5	0.94	0.12	57,61,64,84	0
2	NAD	E	401	44/44	0.95	0.10	35,51,69,72	0
3	PO4	B	402	5/5	0.96	0.11	69,70,74,74	0
3	PO4	D	402	5/5	0.97	0.07	49,51,60,62	0
3	PO4	C	402	5/5	0.98	0.06	56,61,65,69	0
3	PO4	F	402	5/5	0.98	0.10	54,61,80,81	0
3	PO4	G	402	5/5	0.98	0.09	58,59,63,65	0
3	PO4	H	402	5/5	0.98	0.06	40,42,51,55	0

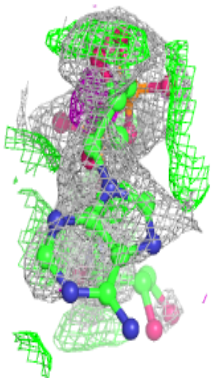
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD F 401:

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

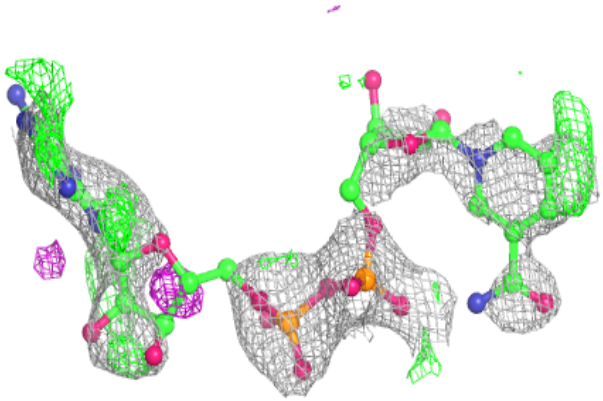


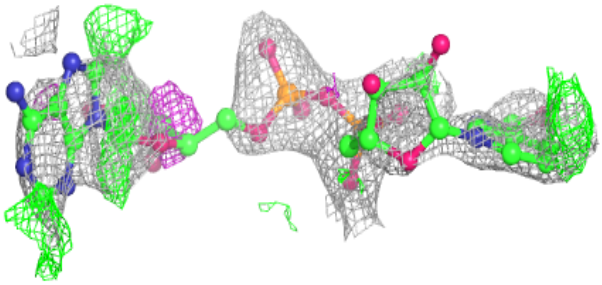


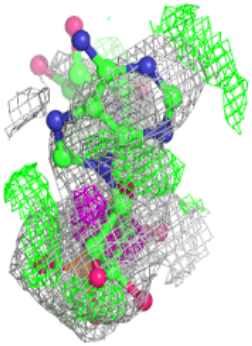


Electron density around NAD B 401:

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

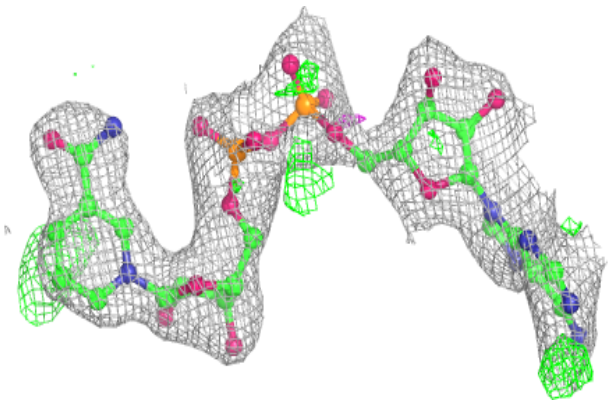


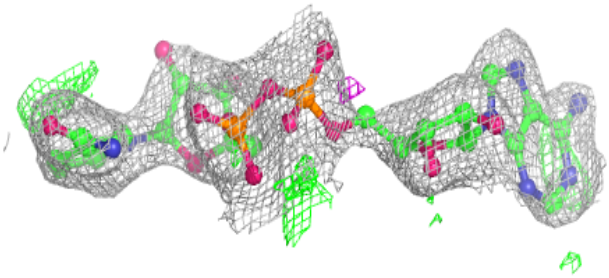


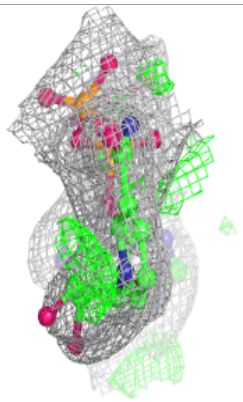


Electron density around NAD D 401:

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

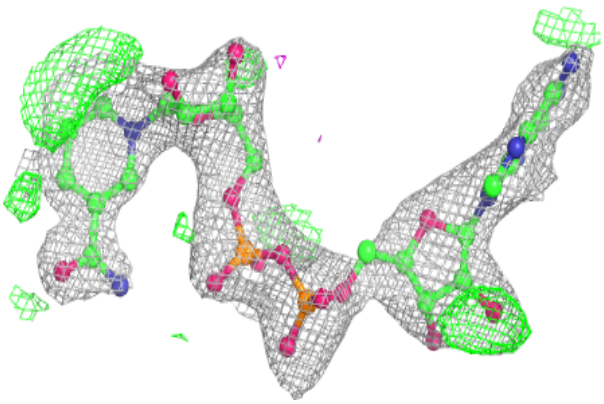


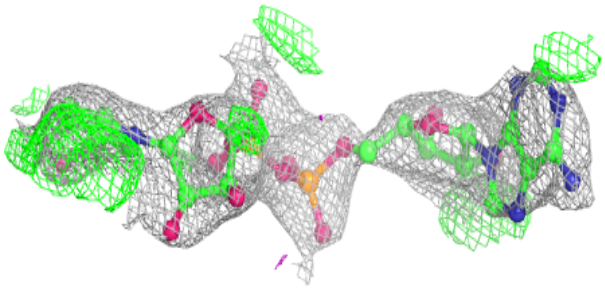


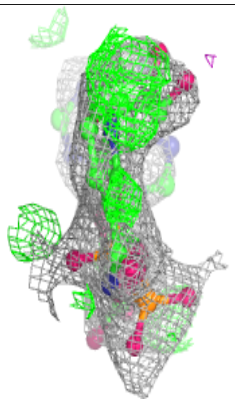


Electron density around NAD G 401:

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

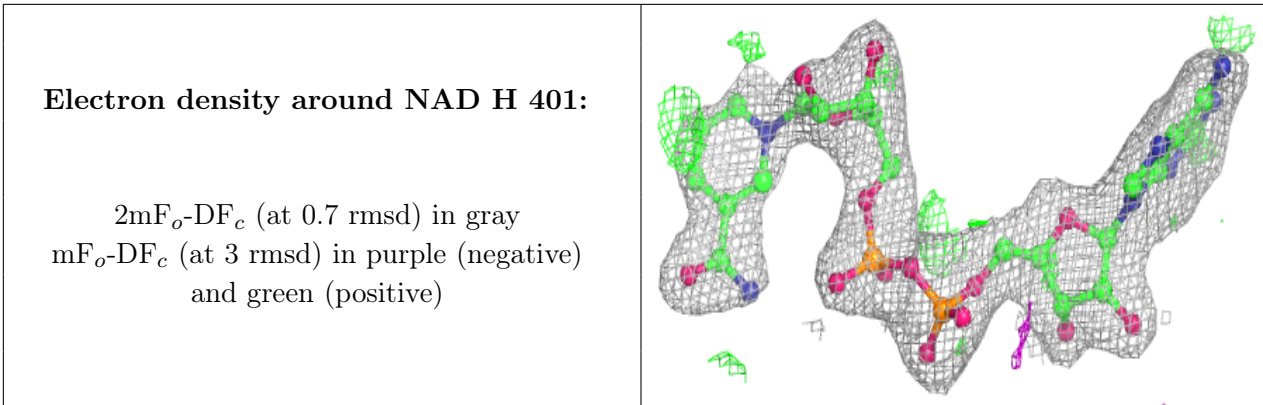


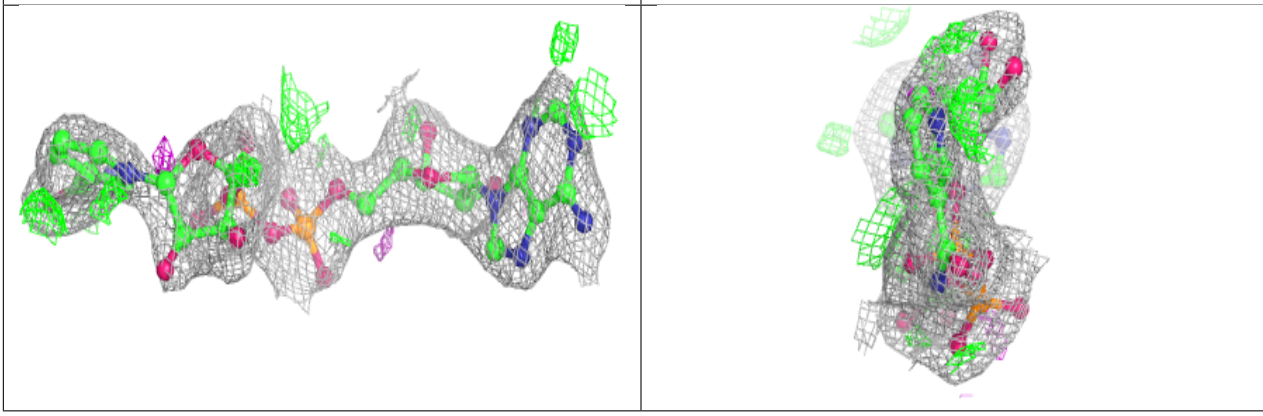




Electron density around NAD H 401:

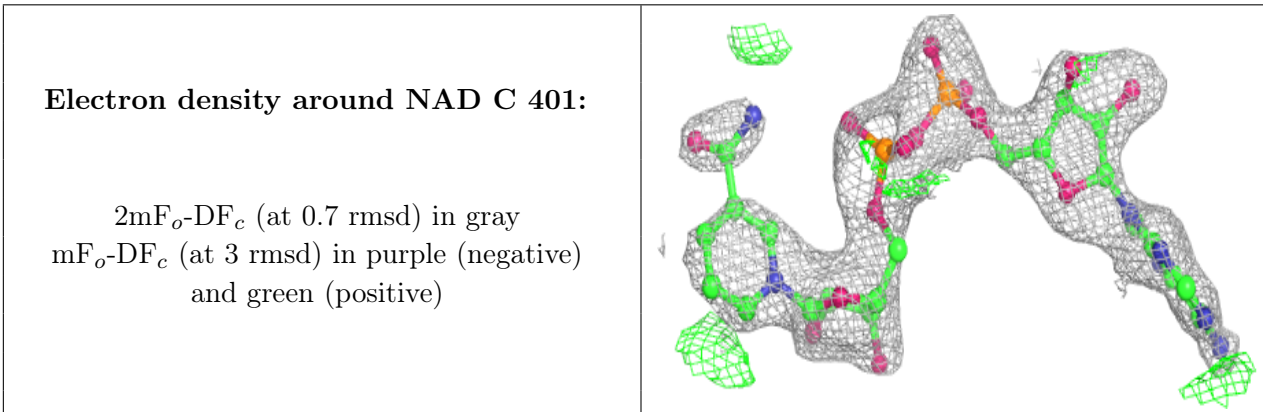
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

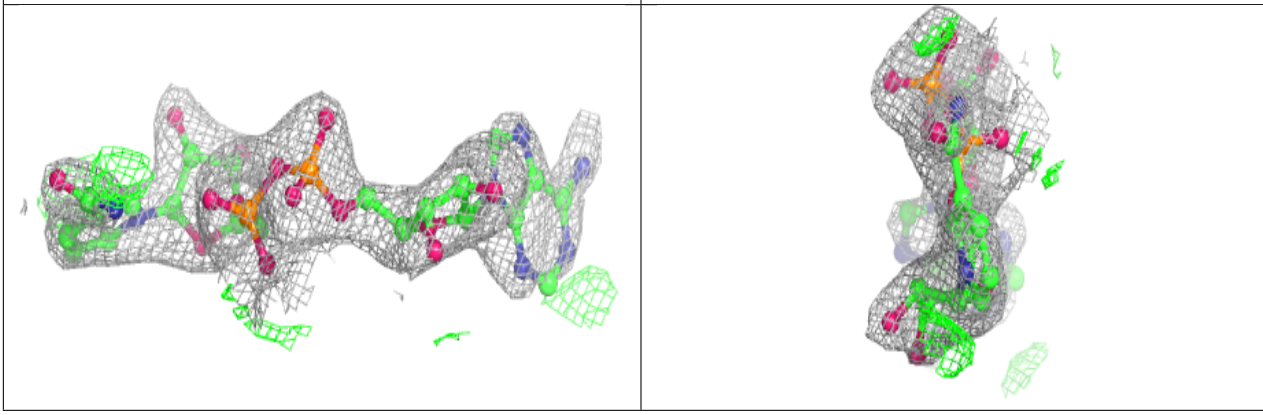




Electron density around NAD C 401:

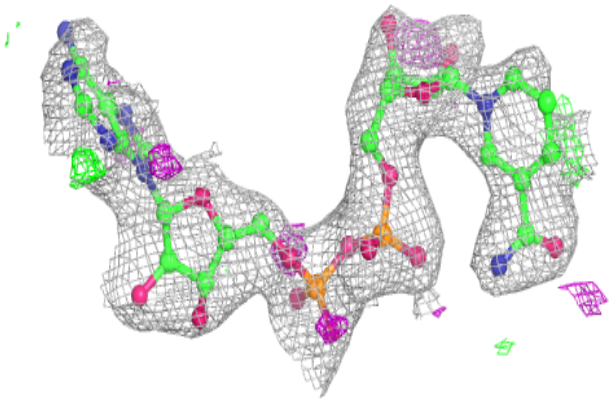
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

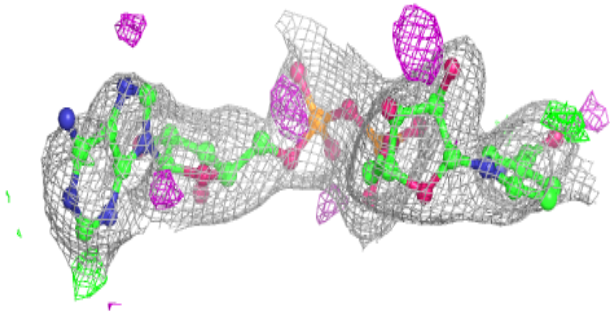


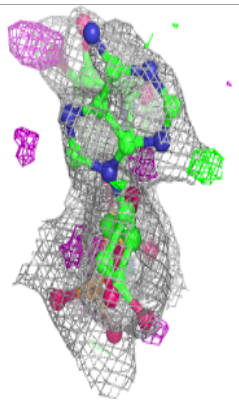


Electron density around NAD A 401:

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

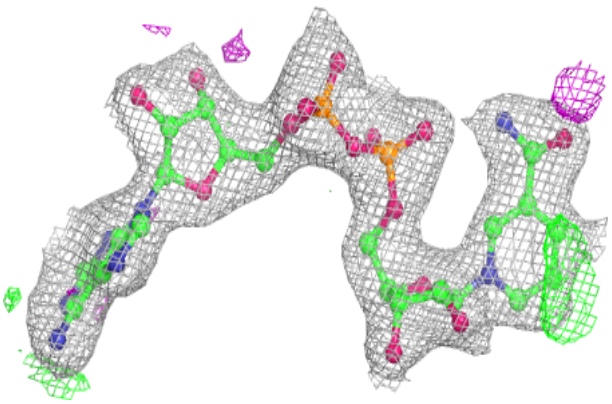


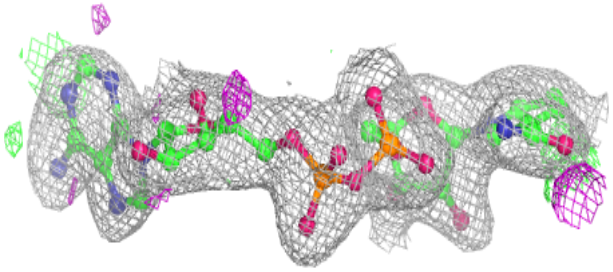


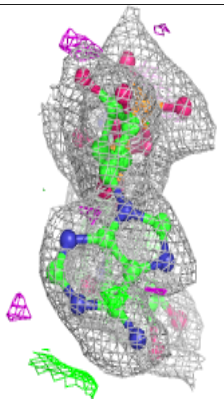


Electron density around NAD E 401:

$2mF_o$-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 (i)

There are no such residues in this entry.