Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:13 am BST

PDB ID	:	3EC7
Title	:	Crystal Structure of Putative Dehydrogenase from Salmonella typhimurium LT2
Authors	:	Kim, Y.; Evdokimova, E.; Kudritska, M.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-08-29
Resolution	:	2.15 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 ⓘ symbol.

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

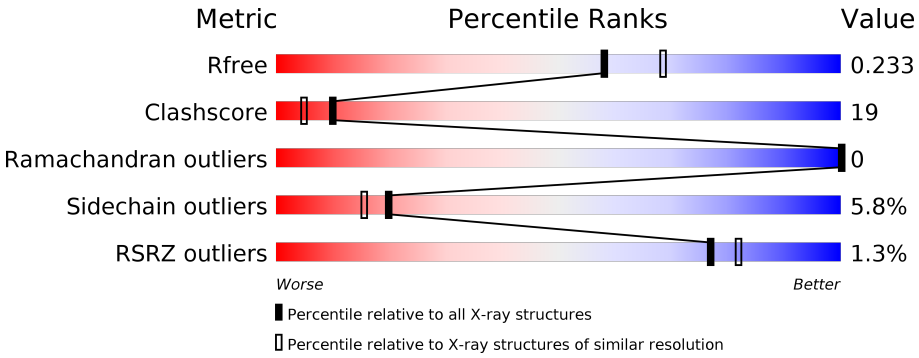
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	357	68% 24% • 6%
1	B	357	2% 67% 24% • 6%
1	C	357	2% 70% 21% • 6%
1	D	357	70% 22% • 6%
1	E	357	71% 21% • 6%
1	F	357	2% 66% 26% • 6%

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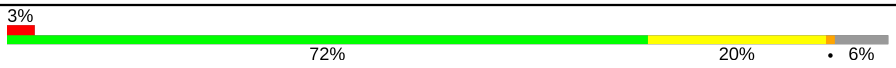
Mol	Chain	Length	Quality of chain
1	G	357	
1	H	357	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23658 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 Putative Dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	Se	0	4	0
			2648	1676	445	513	6	8			
1	B	335	Total	C	N	O	S	Se	0	2	0
			2628	1665	443	506	6	8			
1	C	335	Total	C	N	O	S	Se	0	1	0
			2620	1661	442	504	6	7			
1	D	336	Total	C	N	O	S	Se	0	4	0
			2650	1680	446	510	6	8			
1	E	336	Total	C	N	O	S	Se	0	3	0
			2643	1674	446	510	6	7			
1	F	335	Total	C	N	O	S	Se	0	3	0
			2645	1676	446	508	6	9			
1	G	335	Total	C	N	O	S	Se	0	1	0
			2619	1660	441	504	6	8			
1	H	336	Total	C	N	O	S	Se	0	2	0
			2634	1668	443	510	6	7			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MSE	-	expression tag	UNP Q8ZK57
A	-19	GLY	-	expression tag	UNP Q8ZK57
A	-18	SER	-	expression tag	UNP Q8ZK57
A	-17	SER	-	expression tag	UNP Q8ZK57
A	-16	HIS	-	expression tag	UNP Q8ZK57
A	-15	HIS	-	expression tag	UNP Q8ZK57
A	-14	HIS	-	expression tag	UNP Q8ZK57
A	-13	HIS	-	expression tag	UNP Q8ZK57
A	-12	HIS	-	expression tag	UNP Q8ZK57
A	-11	HIS	-	expression tag	UNP Q8ZK57
A	-10	SER	-	expression tag	UNP Q8ZK57
A	-9	SER	-	expression tag	UNP Q8ZK57
A	-8	GLY	-	expression tag	UNP Q8ZK57

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ARG	-	expression tag	UNP Q8ZK57
A	-6	GLU	-	expression tag	UNP Q8ZK57
A	-5	ASN	-	expression tag	UNP Q8ZK57
A	-4	LEU	-	expression tag	UNP Q8ZK57
A	-3	TYR	-	expression tag	UNP Q8ZK57
A	-2	PHE	-	expression tag	UNP Q8ZK57
A	-1	GLN	-	expression tag	UNP Q8ZK57
A	0	GLY	-	expression tag	UNP Q8ZK57
B	-20	MSE	-	expression tag	UNP Q8ZK57
B	-19	GLY	-	expression tag	UNP Q8ZK57
B	-18	SER	-	expression tag	UNP Q8ZK57
B	-17	SER	-	expression tag	UNP Q8ZK57
B	-16	HIS	-	expression tag	UNP Q8ZK57
B	-15	HIS	-	expression tag	UNP Q8ZK57
B	-14	HIS	-	expression tag	UNP Q8ZK57
B	-13	HIS	-	expression tag	UNP Q8ZK57
B	-12	HIS	-	expression tag	UNP Q8ZK57
B	-11	HIS	-	expression tag	UNP Q8ZK57
B	-10	SER	-	expression tag	UNP Q8ZK57
B	-9	SER	-	expression tag	UNP Q8ZK57
B	-8	GLY	-	expression tag	UNP Q8ZK57
B	-7	ARG	-	expression tag	UNP Q8ZK57
B	-6	GLU	-	expression tag	UNP Q8ZK57
B	-5	ASN	-	expression tag	UNP Q8ZK57
B	-4	LEU	-	expression tag	UNP Q8ZK57
B	-3	TYR	-	expression tag	UNP Q8ZK57
B	-2	PHE	-	expression tag	UNP Q8ZK57
B	-1	GLN	-	expression tag	UNP Q8ZK57
B	0	GLY	-	expression tag	UNP Q8ZK57
C	-20	MSE	-	expression tag	UNP Q8ZK57
C	-19	GLY	-	expression tag	UNP Q8ZK57
C	-18	SER	-	expression tag	UNP Q8ZK57
C	-17	SER	-	expression tag	UNP Q8ZK57
C	-16	HIS	-	expression tag	UNP Q8ZK57
C	-15	HIS	-	expression tag	UNP Q8ZK57
C	-14	HIS	-	expression tag	UNP Q8ZK57
C	-13	HIS	-	expression tag	UNP Q8ZK57
C	-12	HIS	-	expression tag	UNP Q8ZK57
C	-11	HIS	-	expression tag	UNP Q8ZK57
C	-10	SER	-	expression tag	UNP Q8ZK57
C	-9	SER	-	expression tag	UNP Q8ZK57
C	-8	GLY	-	expression tag	UNP Q8ZK57

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ARG	-	expression tag	UNP Q8ZK57
C	-6	GLU	-	expression tag	UNP Q8ZK57
C	-5	ASN	-	expression tag	UNP Q8ZK57
C	-4	LEU	-	expression tag	UNP Q8ZK57
C	-3	TYR	-	expression tag	UNP Q8ZK57
C	-2	PHE	-	expression tag	UNP Q8ZK57
C	-1	GLN	-	expression tag	UNP Q8ZK57
C	0	GLY	-	expression tag	UNP Q8ZK57
D	-20	MSE	-	expression tag	UNP Q8ZK57
D	-19	GLY	-	expression tag	UNP Q8ZK57
D	-18	SER	-	expression tag	UNP Q8ZK57
D	-17	SER	-	expression tag	UNP Q8ZK57
D	-16	HIS	-	expression tag	UNP Q8ZK57
D	-15	HIS	-	expression tag	UNP Q8ZK57
D	-14	HIS	-	expression tag	UNP Q8ZK57
D	-13	HIS	-	expression tag	UNP Q8ZK57
D	-12	HIS	-	expression tag	UNP Q8ZK57
D	-11	HIS	-	expression tag	UNP Q8ZK57
D	-10	SER	-	expression tag	UNP Q8ZK57
D	-9	SER	-	expression tag	UNP Q8ZK57
D	-8	GLY	-	expression tag	UNP Q8ZK57
D	-7	ARG	-	expression tag	UNP Q8ZK57
D	-6	GLU	-	expression tag	UNP Q8ZK57
D	-5	ASN	-	expression tag	UNP Q8ZK57
D	-4	LEU	-	expression tag	UNP Q8ZK57
D	-3	TYR	-	expression tag	UNP Q8ZK57
D	-2	PHE	-	expression tag	UNP Q8ZK57
D	-1	GLN	-	expression tag	UNP Q8ZK57
D	0	GLY	-	expression tag	UNP Q8ZK57
E	-20	MSE	-	expression tag	UNP Q8ZK57
E	-19	GLY	-	expression tag	UNP Q8ZK57
E	-18	SER	-	expression tag	UNP Q8ZK57
E	-17	SER	-	expression tag	UNP Q8ZK57
E	-16	HIS	-	expression tag	UNP Q8ZK57
E	-15	HIS	-	expression tag	UNP Q8ZK57
E	-14	HIS	-	expression tag	UNP Q8ZK57
E	-13	HIS	-	expression tag	UNP Q8ZK57
E	-12	HIS	-	expression tag	UNP Q8ZK57
E	-11	HIS	-	expression tag	UNP Q8ZK57
E	-10	SER	-	expression tag	UNP Q8ZK57
E	-9	SER	-	expression tag	UNP Q8ZK57
E	-8	GLY	-	expression tag	UNP Q8ZK57

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ARG	-	expression tag	UNP Q8ZK57
E	-6	GLU	-	expression tag	UNP Q8ZK57
E	-5	ASN	-	expression tag	UNP Q8ZK57
E	-4	LEU	-	expression tag	UNP Q8ZK57
E	-3	TYR	-	expression tag	UNP Q8ZK57
E	-2	PHE	-	expression tag	UNP Q8ZK57
E	-1	GLN	-	expression tag	UNP Q8ZK57
E	0	GLY	-	expression tag	UNP Q8ZK57
F	-20	MSE	-	expression tag	UNP Q8ZK57
F	-19	GLY	-	expression tag	UNP Q8ZK57
F	-18	SER	-	expression tag	UNP Q8ZK57
F	-17	SER	-	expression tag	UNP Q8ZK57
F	-16	HIS	-	expression tag	UNP Q8ZK57
F	-15	HIS	-	expression tag	UNP Q8ZK57
F	-14	HIS	-	expression tag	UNP Q8ZK57
F	-13	HIS	-	expression tag	UNP Q8ZK57
F	-12	HIS	-	expression tag	UNP Q8ZK57
F	-11	HIS	-	expression tag	UNP Q8ZK57
F	-10	SER	-	expression tag	UNP Q8ZK57
F	-9	SER	-	expression tag	UNP Q8ZK57
F	-8	GLY	-	expression tag	UNP Q8ZK57
F	-7	ARG	-	expression tag	UNP Q8ZK57
F	-6	GLU	-	expression tag	UNP Q8ZK57
F	-5	ASN	-	expression tag	UNP Q8ZK57
F	-4	LEU	-	expression tag	UNP Q8ZK57
F	-3	TYR	-	expression tag	UNP Q8ZK57
F	-2	PHE	-	expression tag	UNP Q8ZK57
F	-1	GLN	-	expression tag	UNP Q8ZK57
F	0	GLY	-	expression tag	UNP Q8ZK57
G	-20	MSE	-	expression tag	UNP Q8ZK57
G	-19	GLY	-	expression tag	UNP Q8ZK57
G	-18	SER	-	expression tag	UNP Q8ZK57
G	-17	SER	-	expression tag	UNP Q8ZK57
G	-16	HIS	-	expression tag	UNP Q8ZK57
G	-15	HIS	-	expression tag	UNP Q8ZK57
G	-14	HIS	-	expression tag	UNP Q8ZK57
G	-13	HIS	-	expression tag	UNP Q8ZK57
G	-12	HIS	-	expression tag	UNP Q8ZK57
G	-11	HIS	-	expression tag	UNP Q8ZK57
G	-10	SER	-	expression tag	UNP Q8ZK57
G	-9	SER	-	expression tag	UNP Q8ZK57
G	-8	GLY	-	expression tag	UNP Q8ZK57

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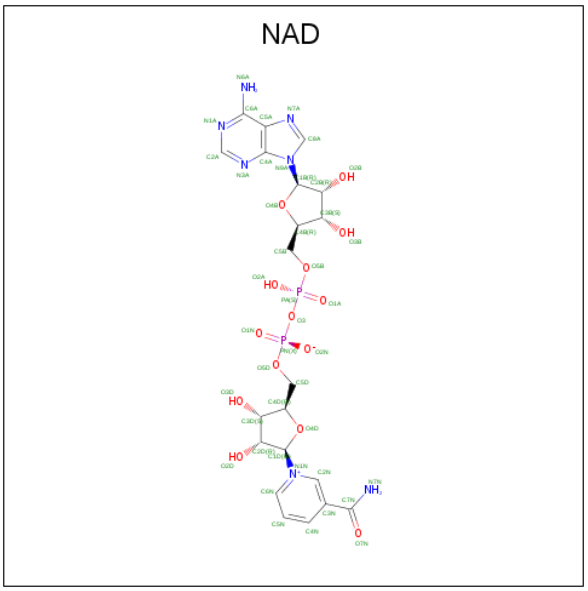
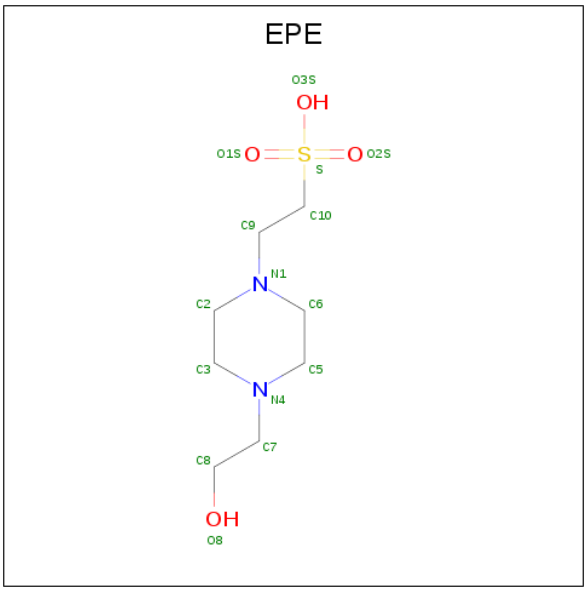
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	ARG	-	expression tag	UNP Q8ZK57
G	-6	GLU	-	expression tag	UNP Q8ZK57
G	-5	ASN	-	expression tag	UNP Q8ZK57
G	-4	LEU	-	expression tag	UNP Q8ZK57
G	-3	TYR	-	expression tag	UNP Q8ZK57
G	-2	PHE	-	expression tag	UNP Q8ZK57
G	-1	GLN	-	expression tag	UNP Q8ZK57
G	0	GLY	-	expression tag	UNP Q8ZK57
H	-20	MSE	-	expression tag	UNP Q8ZK57
H	-19	GLY	-	expression tag	UNP Q8ZK57
H	-18	SER	-	expression tag	UNP Q8ZK57
H	-17	SER	-	expression tag	UNP Q8ZK57
H	-16	HIS	-	expression tag	UNP Q8ZK57
H	-15	HIS	-	expression tag	UNP Q8ZK57
H	-14	HIS	-	expression tag	UNP Q8ZK57
H	-13	HIS	-	expression tag	UNP Q8ZK57
H	-12	HIS	-	expression tag	UNP Q8ZK57
H	-11	HIS	-	expression tag	UNP Q8ZK57
H	-10	SER	-	expression tag	UNP Q8ZK57
H	-9	SER	-	expression tag	UNP Q8ZK57
H	-8	GLY	-	expression tag	UNP Q8ZK57
H	-7	ARG	-	expression tag	UNP Q8ZK57
H	-6	GLU	-	expression tag	UNP Q8ZK57
H	-5	ASN	-	expression tag	UNP Q8ZK57
H	-4	LEU	-	expression tag	UNP Q8ZK57
H	-3	TYR	-	expression tag	UNP Q8ZK57
H	-2	PHE	-	expression tag	UNP Q8ZK57
H	-1	GLN	-	expression tag	UNP Q8ZK57
H	0	GLY	-	expression tag	UNP Q8ZK57

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



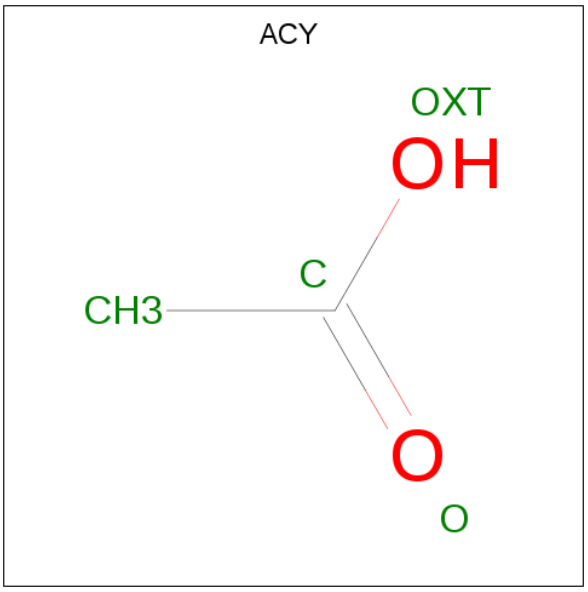
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	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 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



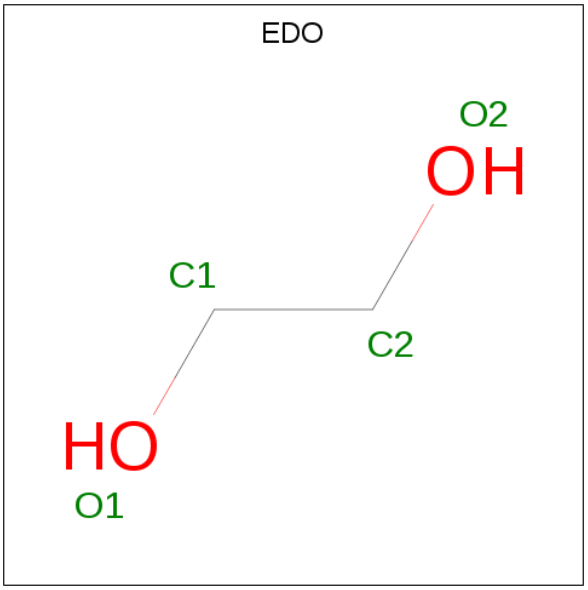
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0

- Molecule 7 is water.

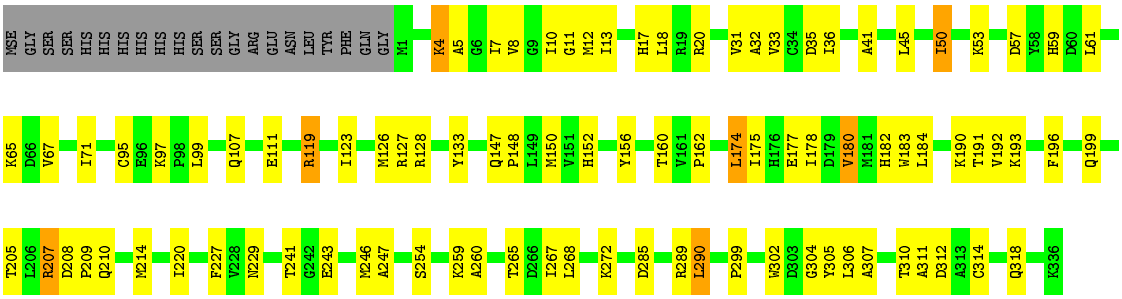
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	321	Total O 321 321	0	0
7	B	264	Total O 264 264	0	0
7	C	226	Total O 226 226	0	0
7	D	260	Total O 260 260	0	0
7	E	282	Total O 282 282	0	0
7	F	231	Total O 231 231	0	0
7	G	219	Total O 219 219	0	0
7	H	266	Total O 266 266	0	0

3 Residue-property plots (i)

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

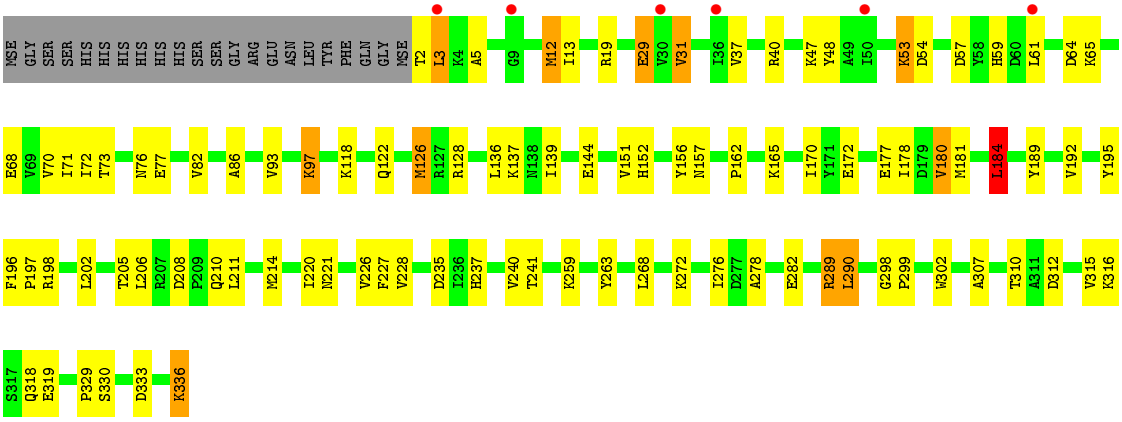
- Molecule 1: Putative Dehydrogenase

Chain A:



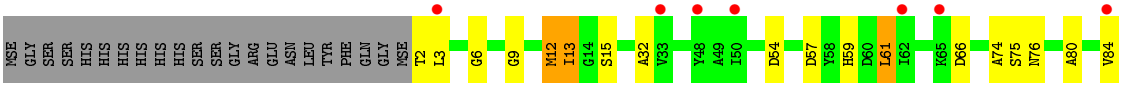
- Molecule 1: Putative Dehydrogenase

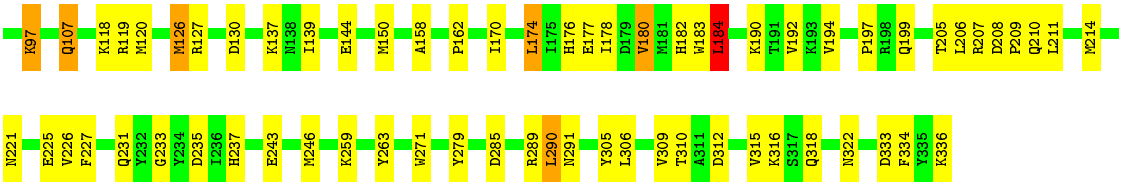
Chain B:



- Molecule 1: Putative Dehydrogenase

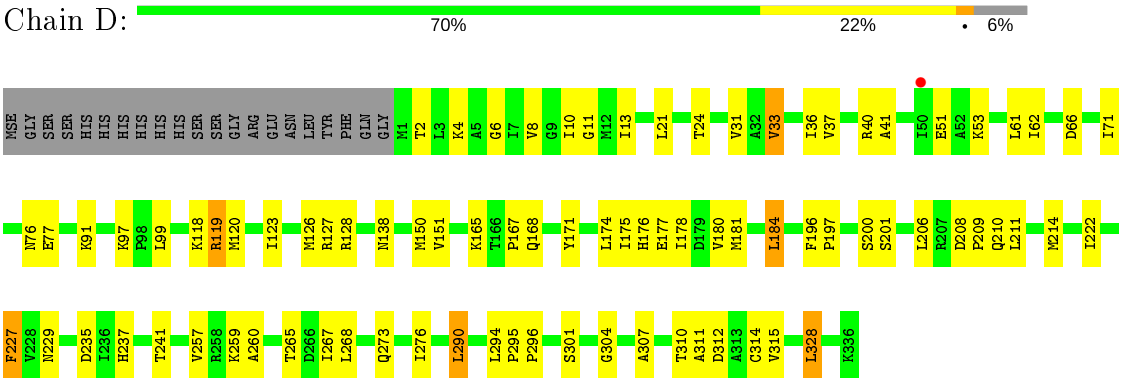
Chain C:





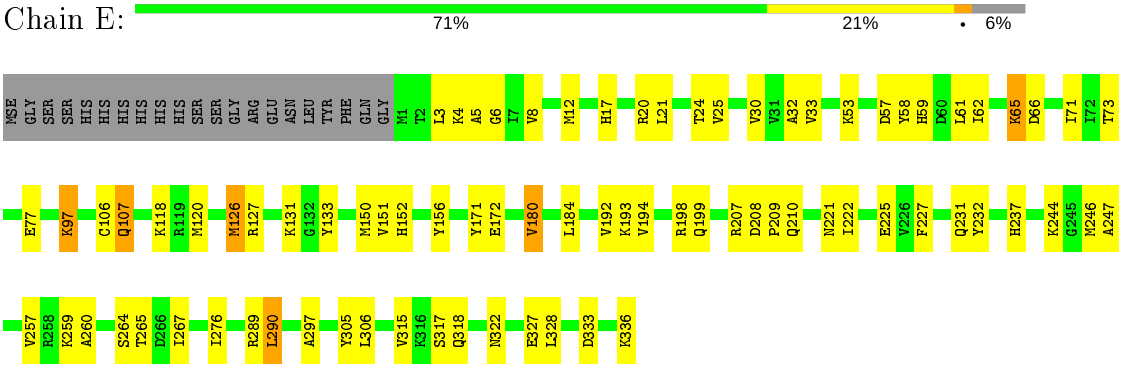
• Molecule 1: Putative Dehydrogenase

Chain D:



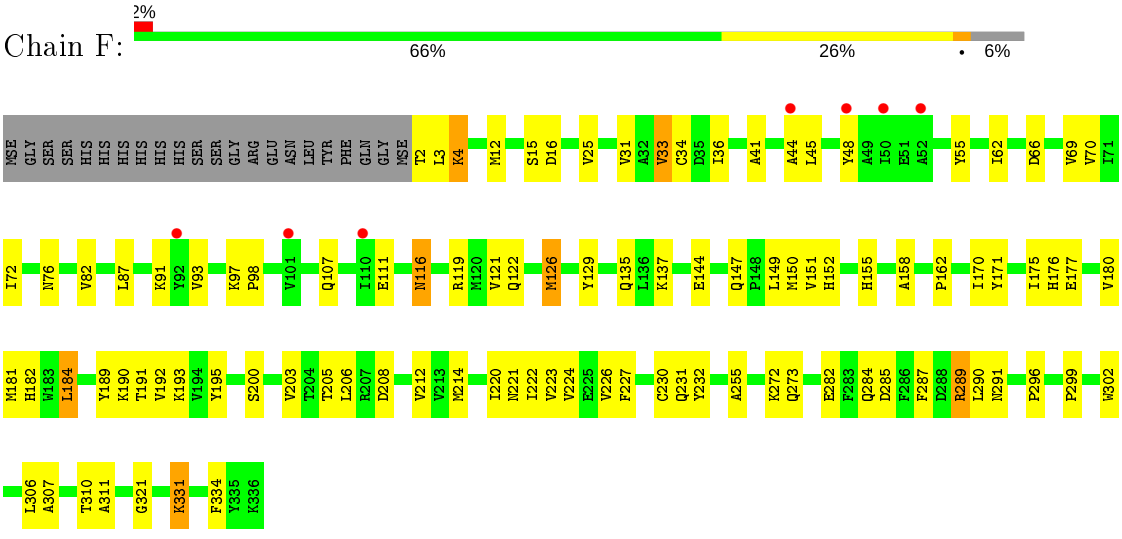
• Molecule 1: Putative Dehydrogenase

Chain E:



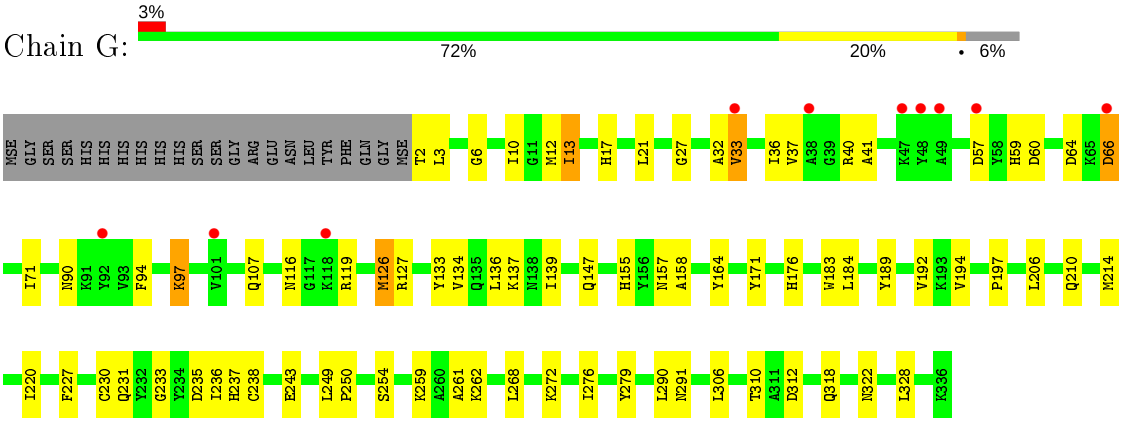
• Molecule 1: Putative Dehydrogenase

Chain F:



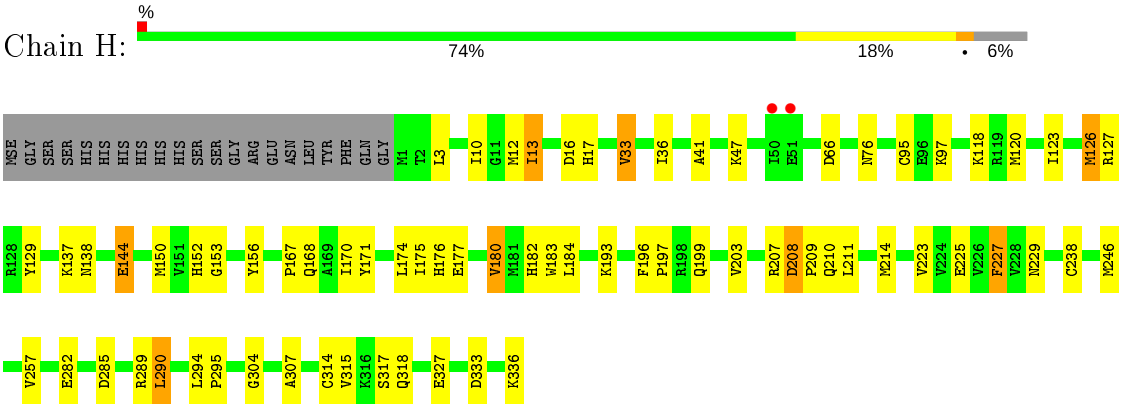
• Molecule 1: Putative Dehydrogenase

Chain G:



• Molecule 1: Putative 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	81.00Å 98.98Å 105.79Å 88.05° 81.78° 89.92°	Depositor
Resolution (Å)	47.00 – 2.15 47.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.00-2.15) 97.8 (47.00-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0053 & phenix.refine	Depositor
R, R_{free}	0.176 , 0.231 0.182 , 0.233	Depositor DCC
R_{free} test set	8685 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.813	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.105 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23658	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: ACY, K, EPE, EDO, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.85	1/2692 (0.0%)	0.81	0/3647
1	B	0.79	0/2672	0.76	2/3620 (0.1%)
1	C	0.74	0/2664	0.76	2/3609 (0.1%)
1	D	0.78	0/2694	0.78	2/3649 (0.1%)
1	E	0.81	0/2687	0.76	0/3640
1	F	0.75	0/2689	0.74	1/3642 (0.0%)
1	G	0.72	1/2663 (0.0%)	0.73	0/3608
1	H	0.78	0/2678	0.76	1/3629 (0.0%)
All	All	0.78	2/21439 (0.0%)	0.76	8/29044 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	TYR	CD1-CE1	7.29	1.50	1.39
1	G	261	ALA	CA-CB	5.54	1.64	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	208	ASP	CB-CG-OD1	7.63	125.17	118.30
1	C	208	ASP	CB-CG-OD1	6.47	124.12	118.30
1	D	208	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	184	LEU	CB-CG-CD1	6.07	121.32	111.00
1	B	208	ASP	CB-CG-OD1	5.95	123.66	118.30
1	F	208	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	184	LEU	CB-CG-CD1	5.82	120.90	111.00
1	C	184	LEU	CB-CG-CD1	5.06	119.60	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	2648	0	2605	118	0
1	B	2628	0	2593	113	0
1	C	2620	0	2590	109	0
1	D	2650	0	2618	114	0
1	E	2643	0	2607	94	0
1	F	2645	0	2615	116	0
1	G	2619	0	2586	93	0
1	H	2634	0	2593	71	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	4	0
2	D	44	0	26	2	0
2	E	44	0	26	0	0
2	F	44	0	26	2	0
2	G	44	0	26	0	0
2	H	44	0	26	1	0
3	A	15	0	18	1	0
3	B	15	0	17	2	0
3	C	15	0	17	2	0
3	D	15	0	17	0	0
3	E	15	0	17	1	0
3	F	15	0	18	0	0
3	G	15	0	18	4	0
3	H	15	0	18	0	0
4	A	8	0	6	1	0
5	D	4	0	6	3	0
5	E	8	0	12	3	0
5	G	4	0	6	3	0
5	H	4	0	6	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
7	A	321	0	0	65	0
7	B	264	0	0	54	0
7	C	226	0	0	56	1
7	D	260	0	0	63	0
7	E	282	0	0	58	1
7	F	231	0	0	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	219	0	0	64	0
7	H	266	0	0	41	0
All	All	23658	0	21191	813	1

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 19.

All (813) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:VAL:HG11	1:D:181:MSE:CE	1.40	1.47
1:C:246:MSE:HG2	7:C:585:HOH:O	1.23	1.32
1:H:210:GLN:HA	7:H:665:HOH:O	1.16	1.31
1:C:176:HIS:HB2	7:C:617:HOH:O	1.28	1.30
1:B:210:GLN:HA	7:B:645:HOH:O	1.32	1.30
2:A:400:NAD:H4B	7:A:694:HOH:O	1.29	1.27
1:D:176:HIS:HA	7:D:625:HOH:O	1.23	1.27
1:F:176:HIS:HB2	7:F:434:HOH:O	1.31	1.27
1:B:226:VAL:HB	7:B:660:HOH:O	1.35	1.26
1:F:158:ALA:HA	7:F:588:HOH:O	1.32	1.26
1:C:150:MSE:CE	1:D:197:PRO:HG2	1.64	1.25
1:F:203:VAL:HG23	7:F:620:HOH:O	1.37	1.25
1:A:193:LYS:HD2	7:A:673:HOH:O	1.34	1.25
1:H:127:ARG:HB3	7:H:639:HOH:O	1.31	1.25
1:B:195:TYR:HB2	7:B:621:HOH:O	1.14	1.24
1:H:214:MSE:HE1	7:H:627:HOH:O	1.14	1.23
1:A:7:ILE:HG22	7:A:723:HOH:O	1.36	1.23
1:A:299:PRO:HA	7:A:719:HOH:O	1.30	1.23
1:D:214:MSE:HE1	7:D:614:HOH:O	1.12	1.22
1:E:246:MSE:HB2	7:F:580:HOH:O	1.32	1.22
1:H:176:HIS:HA	7:H:634:HOH:O	1.33	1.21
1:B:184:LEU:HA	7:B:624:HOH:O	1.41	1.20
1:B:137:LYS:HD3	7:B:624:HOH:O	1.38	1.20
1:C:170:ILE:HB	7:C:612:HOH:O	1.42	1.20
1:D:210:GLN:HA	7:D:626:HOH:O	1.40	1.19
1:H:238:CYS:HA	7:H:669:HOH:O	1.40	1.19
1:C:150:MSE:SE	7:D:654:HOH:O	2.08	1.19
1:A:241:THR:HB	7:A:692:HOH:O	1.39	1.18
1:C:259[B]:LYS:HE3	7:C:600:HOH:O	1.37	1.18
1:A:150:MSE:HB2	7:A:692:HOH:O	1.42	1.18
1:D:151:VAL:CG1	1:D:181:MSE:HE2	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:MSE:CE	1:B:197:PRO:HG2	1.73	1.18
5:G:402:EDO:H21	7:G:779:HOH:O	1.42	1.16
1:A:111[A]:GLU:HG3	7:A:686:HOH:O	1.45	1.16
1:F:193:LYS:HG3	7:F:585:HOH:O	1.46	1.16
1:C:226:VAL:HB	7:C:623:HOH:O	1.45	1.14
1:F:222:ILE:HG22	7:F:584:HOH:O	1.44	1.14
1:E:317:SER:HB2	7:E:797:HOH:O	1.45	1.14
1:C:150:MSE:HE3	1:D:197:PRO:HG2	1.17	1.14
1:G:139:ILE:HD12	7:G:782:HOH:O	1.48	1.13
1:B:139:ILE:HD12	7:B:648:HOH:O	1.47	1.13
1:F:147:GLN:HG3	7:F:616:HOH:O	1.49	1.13
1:H:193:LYS:HD2	7:H:650:HOH:O	1.44	1.13
1:C:158:ALA:HA	7:C:603:HOH:O	1.47	1.12
1:D:123:ILE:HG13	7:D:637:HOH:O	1.45	1.12
1:F:184:LEU:HA	7:F:613:HOH:O	1.49	1.11
1:D:168:GLN:HG2	7:D:458:HOH:O	1.48	1.11
1:D:241:THR:HB	7:D:623:HOH:O	1.49	1.11
1:D:150:MSE:HB2	7:D:623:HOH:O	1.51	1.10
1:C:127:ARG:HD2	7:C:615:HOH:O	1.52	1.09
1:G:13:ILE:HG13	7:G:790:HOH:O	1.50	1.09
1:F:224:VAL:HG23	7:F:584:HOH:O	1.50	1.09
1:C:210:GLN:HB2	7:C:623:HOH:O	1.52	1.08
1:A:150:MSE:HE3	1:B:197:PRO:HG2	1.30	1.08
1:D:151:VAL:HB	7:D:643:HOH:O	1.51	1.08
7:C:596:HOH:O	1:D:200:SER:HA	1.55	1.06
1:H:304:GLY:HA3	7:H:654:HOH:O	1.55	1.06
1:D:151:VAL:CG1	1:D:181:MSE:CE	2.27	1.06
1:B:240:VAL:HG12	7:B:635:HOH:O	1.54	1.06
1:H:225:GLU:HB2	7:H:658:HOH:O	1.56	1.06
1:E:156:TYR:HE1	7:E:771:HOH:O	1.38	1.04
1:A:150:MSE:SE	7:B:548:HOH:O	2.23	1.04
1:C:74:ALA:HB2	7:C:618:HOH:O	1.57	1.04
1:D:311:ALA:HA	7:D:628:HOH:O	1.56	1.04
1:E:267:ILE:HG21	7:E:758:HOH:O	1.56	1.03
1:D:24:THR:HB	7:D:655:HOH:O	1.58	1.03
1:B:31:VAL:O	1:B:53:LYS:HE3	1.57	1.03
1:C:192:VAL:HG12	1:C:214:MSE:HE3	1.38	1.03
1:B:180:VAL:HG22	7:B:620:HOH:O	1.56	1.02
1:H:156:TYR:HE1	7:H:658:HOH:O	1.40	1.02
1:D:167:PRO:HB3	7:D:622:HOH:O	1.59	1.02
1:B:172:GLU:HB3	7:B:640:HOH:O	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HB2	7:B:660:HOH:O	1.57	1.01
3:G:401:EPE:H91	7:G:807:HOH:O	1.59	1.01
1:A:311:ALA:HA	7:A:676:HOH:O	1.58	1.01
1:G:249:LEU:HD22	7:G:791:HOH:O	1.60	1.00
1:A:178:ILE:HD12	7:A:680:HOH:O	1.62	1.00
1:E:225:GLU:HB2	7:E:771:HOH:O	1.63	0.98
1:D:178[B]:ILE:HD11	1:D:307:ALA:HA	1.01	0.98
1:B:37:VAL:HB	1:B:40:ARG:HG3	1.44	0.98
1:D:267:ILE:HG13	7:D:663:HOH:O	1.63	0.98
1:D:178[B]:ILE:HD11	1:D:307:ALA:CA	1.93	0.98
1:H:156:TYR:CE1	7:H:658:HOH:O	2.16	0.98
1:C:184:LEU:HA	7:C:627:HOH:O	1.63	0.97
1:A:207:ARG:HG2	1:A:207:ARG:HH21	1.27	0.97
1:H:168:GLN:HG2	7:H:478:HOH:O	1.65	0.97
1:A:107:GLN:HB2	7:A:705:HOH:O	1.64	0.97
1:B:211:LEU:HB3	7:B:621:HOH:O	1.64	0.97
1:D:328:LEU:HD12	1:D:328:LEU:N	1.80	0.96
7:E:634:HOH:O	1:F:152:HIS:CD2	2.17	0.96
1:G:158:ALA:HA	7:G:811:HOH:O	1.65	0.96
1:D:222:ILE:HG12	7:D:643:HOH:O	1.65	0.96
1:F:70:VAL:HG12	7:F:590:HOH:O	1.64	0.96
1:H:180:VAL:HG21	7:H:639:HOH:O	1.65	0.96
1:G:194:VAL:HG12	7:G:815:HOH:O	1.65	0.95
1:E:4:LYS:HE2	7:E:751:HOH:O	1.67	0.95
1:E:24:THR:HB	7:E:755:HOH:O	1.65	0.95
1:H:197:PRO:HD2	7:H:665:HOH:O	1.66	0.95
1:D:178[B]:ILE:CD1	1:D:307:ALA:HA	1.95	0.95
1:C:150:MSE:HE2	1:D:197:PRO:HG2	1.50	0.94
1:H:229:ASN:HB2	7:H:649:HOH:O	1.66	0.94
1:G:210:GLN:HE22	1:G:318:GLN:HE21	1.15	0.94
1:C:192:VAL:CG1	1:C:214:MSE:HE3	1.97	0.94
1:D:328:LEU:HD11	7:D:491:HOH:O	1.68	0.94
1:D:314:CYS:SG	7:D:628:HOH:O	2.25	0.93
1:A:267:ILE:HG13	7:A:702:HOH:O	1.68	0.93
1:F:149:LEU:HD23	7:F:616:HOH:O	1.68	0.93
1:D:222:ILE:HA	7:D:643:HOH:O	1.68	0.93
1:D:13:ILE:HG12	7:D:607:HOH:O	1.68	0.92
1:G:164:TYR:CD2	7:G:807:HOH:O	2.22	0.92
1:E:107:GLN:HG3	7:E:761:HOH:O	1.69	0.92
1:F:33:VAL:CG2	1:F:41:ALA:HB1	1.98	0.92
1:E:131:LYS:HA	7:E:759:HOH:O	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:HG11	7:A:709:HOH:O	1.71	0.91
1:D:151:VAL:HG11	1:D:181:MSE:HE2	0.93	0.91
1:E:156:TYR:CE1	7:E:771:HOH:O	2.15	0.91
1:F:72:ILE:HG12	7:F:590:HOH:O	1.70	0.91
1:E:246:MSE:HG2	7:E:784:HOH:O	1.68	0.91
1:A:67:VAL:HG21	7:A:684:HOH:O	1.67	0.91
1:A:304:GLY:HA3	7:A:690:HOH:O	1.69	0.91
1:F:184:LEU:HD12	7:F:613:HOH:O	1.70	0.90
1:G:147:GLN:HB3	7:G:802:HOH:O	1.72	0.90
1:D:37:VAL:HB	1:D:40:ARG:HG3	1.52	0.90
1:G:243:GLU:CG	7:G:802:HOH:O	2.19	0.89
1:F:212:VAL:HG23	7:F:627:HOH:O	1.73	0.89
1:G:12[B]:MSE:HE3	1:G:272:LYS:HZ2	1.36	0.89
1:D:178[B]:ILE:HD13	1:D:310:THR:HB	1.54	0.89
1:F:122:GLN:CG	7:F:609:HOH:O	2.19	0.89
1:A:128:ARG:NH1	7:A:719:HOH:O	2.05	0.89
1:A:61:LEU:HG	7:A:684:HOH:O	1.72	0.88
1:G:134:VAL:HA	7:G:798:HOH:O	1.73	0.88
1:D:222:ILE:CG1	7:D:643:HOH:O	2.17	0.87
1:A:150:MSE:HE2	1:B:197:PRO:HG2	1.54	0.87
1:F:311:ALA:HB1	7:F:614:HOH:O	1.72	0.87
1:G:192:VAL:HG12	1:G:214:MSE:HE3	1.56	0.87
1:B:210:GLN:HE22	1:B:318:GLN:HE21	1.19	0.87
1:E:267:ILE:CG2	7:E:758:HOH:O	2.18	0.86
7:E:749:HOH:O	1:F:150:MSE:HE1	1.74	0.86
1:G:158:ALA:HA	7:G:816:HOH:O	1.75	0.86
1:D:229:ASN:HB2	7:D:634:HOH:O	1.74	0.86
1:F:98:PRO:HG2	7:F:587:HOH:O	1.75	0.85
1:D:33:VAL:HG13	1:D:41:ALA:HB1	1.56	0.85
1:B:152:HIS:CD2	7:B:526:HOH:O	2.29	0.85
1:G:279:TYR:CZ	7:G:780:HOH:O	2.28	0.85
1:B:136:LEU:HA	7:B:648:HOH:O	1.76	0.85
1:G:12[B]:MSE:HE3	1:G:272:LYS:NZ	1.92	0.85
1:C:210:GLN:HE22	1:C:318:GLN:HE21	1.25	0.84
1:F:220:ILE:HG22	7:F:598:HOH:O	1.76	0.84
1:B:178:ILE:HG21	7:B:634:HOH:O	1.78	0.84
1:B:72:ILE:HG21	7:B:636:HOH:O	1.78	0.84
1:G:243:GLU:HG3	7:G:802:HOH:O	1.78	0.84
1:G:243:GLU:CD	7:G:802:HOH:O	2.16	0.83
1:C:74:ALA:CB	7:C:618:HOH:O	2.21	0.83
1:B:214:MSE:HE1	1:B:310:THR:HG21	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:PHE:HB2	7:F:629:HOH:O	1.79	0.82
1:E:8:VAL:HG23	7:E:770:HOH:O	1.77	0.82
3:C:401:EPE:H91	7:C:449:HOH:O	1.78	0.82
1:A:214:MSE:HE1	1:A:310:THR:CG2	2.10	0.82
1:F:331[A]:LYS:H	1:F:331[A]:LYS:HE3	1.44	0.82
1:E:25:VAL:HG23	7:E:755:HOH:O	1.78	0.81
1:E:61:LEU:HD22	7:E:770:HOH:O	1.79	0.81
1:A:196:PHE:HD1	7:A:706:HOH:O	1.61	0.81
1:F:137:LYS:HD3	7:F:613:HOH:O	1.79	0.81
1:G:136:LEU:HA	7:G:782:HOH:O	1.79	0.81
1:F:107:GLN:HG3	7:F:581:HOH:O	1.80	0.81
1:G:250:PRO:HG2	5:G:402:EDO:H11	1.63	0.81
1:A:314:CYS:SG	7:A:676:HOH:O	2.37	0.81
1:B:70:VAL:HG11	7:B:619:HOH:O	1.79	0.81
1:A:192:VAL:CG1	1:A:214:MSE:HE3	2.11	0.80
1:C:306:LEU:HB3	7:C:587:HOH:O	1.79	0.80
1:E:231:GLN:HB3	7:E:624:HOH:O	1.81	0.80
1:B:220:ILE:HG22	7:B:617:HOH:O	1.81	0.80
1:E:244:LYS:HE2	7:E:600:HOH:O	1.82	0.80
1:F:170:ILE:HG22	7:F:614:HOH:O	1.81	0.80
1:E:193[B]:LYS:HE2	1:E:194:VAL:N	1.97	0.80
1:F:212:VAL:CG2	7:F:627:HOH:O	2.29	0.79
1:H:211:LEU:HD22	7:H:635:HOH:O	1.82	0.79
7:F:582:HOH:O	1:G:254:SER:HA	1.81	0.79
1:F:25:VAL:HG22	7:F:632:HOH:O	1.82	0.79
7:A:697:HOH:O	1:B:202:LEU:HG	1.83	0.79
1:B:40:ARG:HB3	7:B:626:HOH:O	1.82	0.79
1:F:192:VAL:HG12	1:F:214:MSE:HE3	1.63	0.79
1:B:170:ILE:C	7:B:627:HOH:O	2.20	0.78
1:F:151:VAL:HG12	7:F:586:HOH:O	1.83	0.78
1:G:127:ARG:HD2	7:G:812:HOH:O	1.82	0.78
1:G:279:TYR:CE1	7:G:780:HOH:O	2.34	0.78
1:H:246:MSE:HG2	7:H:432:HOH:O	1.81	0.78
1:E:198:ARG:HD3	7:F:616:HOH:O	1.84	0.78
1:F:122:GLN:HG2	7:F:609:HOH:O	1.81	0.78
1:G:33:VAL:HG13	1:G:41:ALA:HB1	1.65	0.78
1:D:304:GLY:HA3	7:D:608:HOH:O	1.84	0.78
1:G:10:ILE:HD11	1:G:33:VAL:HG22	1.66	0.77
7:G:710:HOH:O	1:H:150:MSE:SE	2.51	0.77
1:A:99:LEU:CD2	7:A:690:HOH:O	2.33	0.77
1:C:150:MSE:CE	1:D:197:PRO:CG	2.55	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:401:EPE:H92	7:E:648:HOH:O	1.85	0.77
3:G:401:EPE:C7	7:G:808:HOH:O	2.32	0.77
1:B:197:PRO:HD3	7:B:645:HOH:O	1.85	0.77
1:D:128:ARG:HB2	7:D:662:HOH:O	1.82	0.77
1:H:167:PRO:HA	7:H:647:HOH:O	1.85	0.76
2:C:400:NAD:H3D	7:C:614:HOH:O	1.85	0.76
7:A:679:HOH:O	1:B:198:ARG:HD2	1.84	0.76
1:C:9:GLY:HA3	7:C:618:HOH:O	1.86	0.76
1:F:192:VAL:CG1	1:F:214:MSE:HE3	2.16	0.76
1:A:192:VAL:CG1	1:A:214:MSE:CE	2.64	0.76
1:B:72:ILE:HD13	7:B:636:HOH:O	1.85	0.76
1:C:144:GLU:OE1	7:C:554:HOH:O	2.04	0.76
1:C:150:MSE:HE2	1:D:197:PRO:CG	2.15	0.76
1:D:99:LEU:CD2	7:D:608:HOH:O	2.34	0.76
3:G:401:EPE:H72	7:G:808:HOH:O	1.85	0.76
1:B:189:TYR:CD1	1:B:214:MSE:HE2	2.20	0.75
1:A:192:VAL:HG11	1:A:214:MSE:HE3	1.69	0.75
1:A:305:TYR:HE2	7:A:705:HOH:O	1.69	0.75
1:B:178:ILE:HD13	7:B:634:HOH:O	1.86	0.74
1:A:99:LEU:HD23	7:A:690:HOH:O	1.87	0.74
1:C:259[B]:LYS:CE	7:C:600:HOH:O	2.11	0.74
1:F:299:PRO:HD2	7:F:609:HOH:O	1.87	0.74
1:G:126:MSE:SE	7:G:780:HOH:O	2.54	0.74
1:A:11:GLY:N	7:A:694:HOH:O	2.20	0.74
1:D:151:VAL:HG11	1:D:181:MSE:HE3	1.65	0.74
1:D:196:PHE:HA	7:D:626:HOH:O	1.87	0.74
1:A:150:MSE:CE	1:B:197:PRO:CG	2.63	0.73
1:E:30:VAL:CG1	7:E:781:HOH:O	2.34	0.73
1:B:220:ILE:CG2	7:B:617:HOH:O	2.36	0.73
1:F:220:ILE:CG2	7:F:598:HOH:O	2.33	0.73
1:A:147:GLN:NE2	7:A:685:HOH:O	2.22	0.73
1:F:122:GLN:HG3	7:F:609:HOH:O	1.86	0.73
1:A:192:VAL:HG12	1:A:214:MSE:CE	2.19	0.73
1:E:150:MSE:HE1	7:F:591:HOH:O	1.88	0.73
1:D:222:ILE:CA	7:D:643:HOH:O	2.29	0.73
1:A:12[B]:MSE:HE3	1:A:272:LYS:NZ	2.03	0.73
1:E:33:VAL:HG13	7:E:781:HOH:O	1.89	0.73
1:A:207:ARG:NH2	7:A:419:HOH:O	2.21	0.72
1:A:199:GLN:HE22	1:A:207:ARG:HA	1.54	0.72
1:C:194:VAL:HG13	7:C:601:HOH:O	1.88	0.72
1:H:123:ILE:HG13	7:H:654:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:VAL:HG22	7:H:647:HOH:O	1.87	0.72
1:B:210:GLN:NE2	1:B:318:GLN:HE21	1.86	0.72
1:B:259:LYS:HE3	1:E:327[A]:GLU:OE2	1.90	0.72
1:B:165:LYS:HE3	7:B:478:HOH:O	1.90	0.71
1:E:264:SER:HB2	7:E:768:HOH:O	1.89	0.71
1:G:231:GLN:N	7:G:816:HOH:O	2.23	0.71
1:G:97:LYS:HE2	1:G:176:HIS:CE1	2.25	0.71
1:E:246:MSE:HE3	7:F:580:HOH:O	1.89	0.71
1:G:189:TYR:CD1	1:G:214:MSE:HE2	2.26	0.71
1:H:210:GLN:HE22	1:H:318:GLN:HE21	1.36	0.71
1:B:29:GLU:HB3	7:B:643:HOH:O	1.89	0.71
1:F:192:VAL:HG11	7:F:601:HOH:O	1.91	0.71
1:G:37:VAL:HB	1:G:40:ARG:HG3	1.73	0.71
1:C:174:LEU:O	1:C:174:LEU:HD23	1.90	0.70
1:D:150:MSE:CB	7:D:623:HOH:O	2.22	0.70
1:B:192:VAL:HG12	1:B:214:MSE:HE3	1.72	0.70
1:A:207:ARG:CG	1:A:207:ARG:HH21	2.00	0.70
1:D:227:PHE:CE1	7:D:634:HOH:O	2.44	0.70
1:F:195:TYR:CD2	7:F:585:HOH:O	2.45	0.70
1:G:158:ALA:CB	7:G:811:HOH:O	2.38	0.70
1:F:311:ALA:CB	7:F:614:HOH:O	2.35	0.70
1:A:210:GLN:HG2	7:A:706:HOH:O	1.91	0.69
1:B:126:MSE:CE	7:B:638:HOH:O	2.41	0.69
1:B:211:LEU:HD12	7:B:621:HOH:O	1.90	0.69
1:C:150:MSE:HE2	1:D:211:LEU:HB2	1.73	0.69
1:G:194:VAL:CG1	7:G:815:HOH:O	2.32	0.69
1:G:237:HIS:HD2	7:G:695:HOH:O	1.74	0.69
1:A:209:PRO:O	7:A:706:HOH:O	2.10	0.68
1:A:150:MSE:HE2	1:B:197:PRO:CG	2.23	0.68
1:E:152:HIS:CD2	7:E:634:HOH:O	2.45	0.68
1:F:310:THR:O	7:F:601:HOH:O	2.10	0.68
1:A:193:LYS:O	7:A:681:HOH:O	2.12	0.68
1:G:59:HIS:HB2	7:G:667:HOH:O	1.93	0.68
1:H:171:TYR:CZ	1:H:315:VAL:HG21	2.28	0.68
1:B:31:VAL:O	1:B:53:LYS:CE	2.38	0.68
1:A:10:ILE:HG13	1:A:33:VAL:HG13	1.76	0.68
1:H:203:VAL:HG21	7:H:649:HOH:O	1.93	0.67
1:D:197:PRO:HD2	7:D:626:HOH:O	1.93	0.67
1:D:273:GLN:HG3	7:D:513:HOH:O	1.94	0.67
1:A:285:ASP:O	1:A:289:ARG:HG3	1.93	0.67
1:E:317:SER:CB	7:E:797:HOH:O	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HG12	7:B:528:HOH:O	1.93	0.67
1:B:144:GLU:HG2	1:C:259[A]:LYS:HE2	1.75	0.67
1:E:192:VAL:HG23	7:E:797:HOH:O	1.93	0.67
1:E:30:VAL:HG12	7:E:781:HOH:O	1.95	0.67
1:C:180:VAL:CG2	7:C:610:HOH:O	2.43	0.66
1:E:289:ARG:HD3	7:E:571:HOH:O	1.93	0.66
1:H:153:GLY:HA2	7:H:669:HOH:O	1.95	0.66
1:E:106:CYS:HB3	7:E:752:HOH:O	1.95	0.66
1:H:152:HIS:O	7:H:669:HOH:O	2.14	0.66
1:A:193:LYS:HG3	7:A:681:HOH:O	1.94	0.66
1:F:230:CYS:SG	7:F:588:HOH:O	2.52	0.66
1:H:209:PRO:O	7:H:662:HOH:O	2.14	0.66
1:B:214:MSE:HE1	1:B:310:THR:CG2	2.24	0.66
1:E:265:THR:O	7:E:768:HOH:O	2.14	0.66
1:G:107:GLN:HB3	7:G:646:HOH:O	1.95	0.66
1:B:210:GLN:HE22	1:B:318:GLN:NE2	1.90	0.66
1:E:222:ILE:CG1	7:E:795:HOH:O	2.43	0.66
1:A:247:ALA:O	7:A:470:HOH:O	2.13	0.66
1:A:150:MSE:HE2	1:B:211:LEU:HB2	1.77	0.66
1:B:59:HIS:HE1	7:B:618:HOH:O	1.78	0.66
1:C:197:PRO:HG2	7:C:598:HOH:O	1.96	0.66
1:G:183:TRP:CH2	7:G:798:HOH:O	2.47	0.66
1:E:305:TYR:HB2	7:E:752:HOH:O	1.96	0.66
1:F:189:TYR:CD1	1:F:214:MSE:HE2	2.31	0.66
1:A:192:VAL:HG11	1:A:214:MSE:CE	2.26	0.66
1:A:193:LYS:CD	7:A:673:HOH:O	2.11	0.65
1:D:328:LEU:HD12	1:D:328:LEU:H	1.58	0.65
1:E:180:VAL:CG1	7:E:769:HOH:O	2.43	0.65
1:E:257:VAL:HG23	5:E:402:EDO:H11	1.76	0.65
1:B:86:ALA:HB2	7:B:619:HOH:O	1.96	0.65
1:C:75:SER:HA	7:C:614:HOH:O	1.95	0.65
1:E:222:ILE:HG13	7:E:795:HOH:O	1.96	0.65
1:F:144:GLU:CG	1:G:259:LYS:HE2	2.27	0.65
1:G:230:CYS:SG	7:G:816:HOH:O	2.54	0.65
1:F:184:LEU:CD1	7:F:613:HOH:O	2.33	0.65
1:D:304:GLY:HA3	7:D:637:HOH:O	1.96	0.65
1:A:305:TYR:CE2	7:A:705:HOH:O	2.48	0.65
1:B:184:LEU:CD1	7:B:624:HOH:O	2.44	0.65
1:G:192:VAL:CG1	1:G:214:MSE:HE3	2.27	0.65
1:A:205:THR:HB	7:A:715:HOH:O	1.94	0.65
1:B:196:PHE:HA	7:B:645:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:VAL:HG12	1:C:214:MSE:CE	2.21	0.65
1:E:289:ARG:HH11	1:E:297:ALA:HB3	1.62	0.65
1:A:162:PRO:O	7:A:715:HOH:O	2.14	0.65
1:C:107:GLN:NE2	1:C:305:TYR:CE2	2.65	0.65
1:C:174:LEU:HD22	1:C:178:ILE:HG13	1.78	0.65
1:E:8:VAL:CG2	7:E:770:HOH:O	2.42	0.65
1:F:224:VAL:HG13	7:F:607:HOH:O	1.96	0.65
1:A:192:VAL:HG12	1:A:214:MSE:HE2	1.79	0.65
1:F:119:ARG:HG3	1:F:334:PHE:CE2	2.32	0.65
1:C:9:GLY:CA	7:C:618:HOH:O	2.45	0.64
1:E:289:ARG:NH1	1:E:297:ALA:HB3	2.12	0.64
1:F:151:VAL:HG23	7:F:598:HOH:O	1.97	0.64
1:C:243:GLU:OE2	7:C:596:HOH:O	2.15	0.64
1:B:307:ALA:O	7:B:634:HOH:O	2.15	0.64
1:D:119:ARG:HG2	7:D:633:HOH:O	1.97	0.64
1:F:12[C]:MSE:HE3	1:F:272:LYS:NZ	2.12	0.64
1:F:181:MSE:HE1	7:F:586:HOH:O	1.96	0.64
1:D:265:THR:HA	5:D:402:EDO:H21	1.79	0.64
1:A:174:LEU:HB3	7:A:680:HOH:O	1.98	0.64
1:D:227:PHE:HE1	7:D:634:HOH:O	1.78	0.64
1:C:184:LEU:CD1	7:C:627:HOH:O	2.46	0.64
1:A:243:GLU:OE1	7:A:697:HOH:O	2.15	0.64
1:A:12[B]:MSE:HE3	1:A:272:LYS:HZ2	1.63	0.64
1:H:47:LYS:HD3	7:H:663:HOH:O	1.97	0.64
1:C:285:ASP:OD1	1:C:289:ARG:NH1	2.32	0.63
1:D:77[B]:GLU:H	1:D:77[B]:GLU:CD	2.01	0.63
1:E:199:GLN:HE22	1:E:207:ARG:HA	1.63	0.63
1:F:214:MSE:HE1	1:F:310:THR:HG21	1.80	0.63
1:F:33:VAL:HG22	1:F:41:ALA:HB1	1.79	0.63
7:C:593:HOH:O	1:D:150:MSE:HE1	1.97	0.63
1:B:235:ASP:OD2	1:B:237:HIS:HE1	1.82	0.63
1:F:12[B]:MSE:SE	1:F:272:LYS:HZ3	2.32	0.63
1:C:184:LEU:HD13	7:C:627:HOH:O	1.99	0.63
1:B:12[A]:MSE:CE	7:B:616:HOH:O	2.47	0.63
1:B:82:VAL:HG12	7:B:619:HOH:O	1.97	0.62
1:D:197:PRO:CD	7:D:626:HOH:O	2.47	0.62
1:A:150:MSE:HE3	1:B:197:PRO:CG	2.19	0.62
1:C:76:ASN:N	7:C:614:HOH:O	2.32	0.62
1:F:331[A]:LYS:H	1:F:331[A]:LYS:CE	2.10	0.62
1:F:3:LEU:HD11	1:F:290:LEU:HB3	1.82	0.62
1:E:118:LYS:HG2	7:E:779:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135[B]:GLN:CD	7:F:582:HOH:O	2.36	0.62
1:H:76:ASN:ND2	2:H:400:NAD:O3D	2.32	0.62
1:E:244:LYS:CE	7:E:600:HOH:O	2.43	0.62
1:B:12[A]:MSE:HE3	1:B:272:LYS:NZ	2.15	0.62
1:C:158:ALA:CB	7:C:603:HOH:O	2.47	0.62
1:F:144:GLU:HG3	1:G:259:LYS:HE2	1.81	0.62
1:C:246:MSE:CG	7:C:585:HOH:O	2.02	0.61
1:D:171:TYR:CE2	7:D:622:HOH:O	2.51	0.61
1:D:237:HIS:HD2	7:D:615:HOH:O	1.82	0.61
1:H:199:GLN:HE22	1:H:207:ARG:HA	1.64	0.61
1:E:232:TYR:HE1	7:E:758:HOH:O	1.83	0.61
1:E:57:ASP:OD1	1:E:59:HIS:HD2	1.82	0.61
1:A:304:GLY:CA	7:A:690:HOH:O	2.38	0.60
1:B:151:VAL:HG23	7:B:617:HOH:O	2.00	0.60
1:H:210:GLN:NE2	1:H:318:GLN:HE21	2.00	0.60
1:G:133:TYR:O	7:G:798:HOH:O	2.15	0.60
1:F:12[C]:MSE:CE	7:F:589:HOH:O	2.50	0.60
1:H:33:VAL:HG13	1:H:41:ALA:HB1	1.83	0.60
1:A:57:ASP:OD2	1:A:59:HIS:HD2	1.85	0.60
1:B:195:TYR:O	7:B:645:HOH:O	2.16	0.60
1:C:97:LYS:NZ	1:C:176:HIS:NE2	2.43	0.60
1:F:289:ARG:HD3	7:F:474:HOH:O	2.00	0.60
1:C:210:GLN:NE2	1:C:318:GLN:HE21	1.98	0.60
1:A:210:GLN:HE22	1:A:318:GLN:HE21	1.50	0.59
1:A:57:ASP:OD2	1:A:59:HIS:CD2	2.54	0.59
1:B:197:PRO:CD	7:B:645:HOH:O	2.45	0.59
1:A:312:ASP:OD2	4:A:402:ACY:H3	2.02	0.59
1:C:243:GLU:HG2	7:C:596:HOH:O	2.02	0.59
1:E:58:TYR:O	1:E:62:ILE:HG12	2.02	0.59
1:F:284:GLN:HA	7:F:629:HOH:O	2.01	0.59
1:A:207:ARG:HG2	1:A:207:ARG:NH2	2.02	0.59
1:F:12[B]:MSE:SE	1:F:272:LYS:NZ	2.86	0.59
1:H:10:ILE:HD11	1:H:33:VAL:HG22	1.83	0.59
1:C:199:GLN:HE22	1:C:207:ARG:HA	1.67	0.59
1:C:3:LEU:HG	1:C:291:ASN:ND2	2.17	0.59
1:D:151:VAL:CG1	1:D:181:MSE:HE1	2.23	0.59
7:C:596:HOH:O	1:D:201:SER:N	2.28	0.59
1:F:151:VAL:CG1	7:F:586:HOH:O	2.45	0.59
1:E:66:ASP:HA	7:E:644:HOH:O	2.01	0.59
1:E:237:HIS:HD2	7:E:654:HOH:O	1.86	0.59
1:A:33:VAL:HG12	1:A:41:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD22	7:D:608:HOH:O	1.97	0.58
1:C:61:LEU:C	1:C:61:LEU:HD13	2.24	0.58
1:D:8:VAL:HG23	7:D:641:HOH:O	2.03	0.58
1:E:71:ILE:N	1:E:71:ILE:HD12	2.18	0.58
1:F:192:VAL:HG21	7:F:601:HOH:O	2.03	0.58
1:A:4:LYS:HG2	1:A:31:VAL:HG11	1.85	0.58
1:A:148:PRO:HD2	7:A:685:HOH:O	2.03	0.58
1:B:289:ARG:HH11	1:B:289:ARG:HG3	1.67	0.58
1:F:231:GLN:N	7:F:588:HOH:O	2.35	0.58
1:D:290:LEU:HD11	1:D:296:PRO:HD3	1.84	0.58
1:E:225:GLU:O	7:E:771:HOH:O	2.17	0.58
1:A:310:THR:HG23	7:A:709:HOH:O	2.04	0.58
1:B:184:LEU:HD12	7:B:624:HOH:O	2.03	0.58
1:E:127:ARG:HD2	7:E:769:HOH:O	2.02	0.58
1:G:36:ILE:HD11	7:G:773:HOH:O	2.04	0.57
1:B:316:LYS:NZ	7:B:582:HOH:O	2.38	0.57
1:B:31:VAL:HG13	7:B:643:HOH:O	2.05	0.57
1:E:210:GLN:HE22	1:E:318:GLN:HE21	1.50	0.57
1:H:210:GLN:HE22	1:H:318:GLN:NE2	2.02	0.57
1:C:150:MSE:HE3	1:D:197:PRO:CG	2.12	0.57
1:H:304:GLY:CA	7:H:654:HOH:O	2.30	0.57
1:H:3:LEU:HD11	1:H:290:LEU:HB3	1.85	0.57
1:D:304:GLY:CA	7:D:637:HOH:O	2.52	0.57
1:G:33:VAL:CG1	1:G:41:ALA:HB1	2.33	0.57
1:A:314:CYS:HB2	7:A:676:HOH:O	2.05	0.57
1:B:57:ASP:OD2	1:B:59:HIS:HD2	1.87	0.57
1:C:333:ASP:HA	1:C:336:LYS:HG3	1.87	0.57
1:G:158:ALA:CA	7:G:811:HOH:O	2.34	0.57
1:B:5:ALA:HB1	1:B:71:ILE:HD13	1.86	0.57
1:C:3:LEU:HG	1:C:291:ASN:HD21	1.69	0.57
1:G:137:LYS:CB	7:G:798:HOH:O	2.52	0.57
1:D:314:CYS:HB2	7:D:628:HOH:O	2.05	0.57
1:D:304:GLY:CA	7:D:608:HOH:O	2.47	0.56
1:H:317:SER:OG	7:H:650:HOH:O	2.18	0.56
1:C:150:MSE:HE1	1:D:210:GLN:O	2.05	0.56
1:G:176:HIS:HB3	7:G:812:HOH:O	2.06	0.56
1:B:192:VAL:CG1	1:B:214:MSE:HE3	2.35	0.56
1:E:244:LYS:NZ	7:E:600:HOH:O	2.37	0.56
1:E:247:ALA:O	7:E:784:HOH:O	2.17	0.56
7:A:679:HOH:O	1:B:198:ARG:HB2	2.05	0.56
1:D:99:LEU:HD23	7:D:608:HOH:O	1.98	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HD21	1:B:290:LEU:HB3	1.87	0.56
1:H:175:ILE:HD11	1:H:307:ALA:HB1	1.87	0.56
1:C:150:MSE:HE3	1:D:209:PRO:HG2	1.88	0.56
1:A:127:ARG:NH1	7:A:711:HOH:O	2.38	0.56
1:D:328:LEU:CD1	1:D:328:LEU:N	2.60	0.56
1:H:227:PHE:HE1	7:H:649:HOH:O	1.88	0.56
1:A:192:VAL:CG1	1:A:214:MSE:HE2	2.35	0.56
1:E:225:GLU:CB	7:E:771:HOH:O	2.35	0.56
1:G:157:ASN:O	7:G:816:HOH:O	2.18	0.55
1:G:220:ILE:HG22	7:G:785:HOH:O	2.04	0.55
1:F:289:ARG:CD	7:F:474:HOH:O	2.55	0.55
1:H:285:ASP:OD1	1:H:289:ARG:NH1	2.38	0.55
1:C:3:LEU:HD11	1:C:290:LEU:HB3	1.88	0.55
1:C:192:VAL:HG11	1:C:214:MSE:HE3	1.87	0.55
1:E:65:LYS:HD3	1:E:65:LYS:O	2.06	0.55
1:G:230:CYS:N	7:G:816:HOH:O	2.39	0.55
1:E:193[B]:LYS:CE	1:E:317:SER:OG	2.55	0.55
1:F:200:SER:OG	7:F:620:HOH:O	2.18	0.55
1:H:196:PHE:HA	7:H:665:HOH:O	2.07	0.55
1:C:144:GLU:HG3	1:E:327[B]:GLU:OE1	2.05	0.55
1:C:209:PRO:HB2	7:C:598:HOH:O	2.06	0.55
1:B:278:ALA:O	1:B:282:GLU:HG2	2.06	0.55
1:E:5:ALA:HB1	1:E:71:ILE:CD1	2.37	0.55
1:C:12:MSE:HG3	1:C:13:ILE:N	2.22	0.55
1:C:214:MSE:HE1	1:C:310:THR:CG2	2.37	0.55
1:C:180:VAL:HG21	7:C:610:HOH:O	2.07	0.54
1:H:13:ILE:HG13	7:H:631:HOH:O	2.06	0.54
1:A:128:ARG:CZ	7:A:719:HOH:O	2.49	0.54
1:B:72:ILE:HD12	1:B:93:VAL:HG13	1.90	0.54
1:D:62:ILE:O	1:D:91:LYS:NZ	2.38	0.54
1:A:196:PHE:CD1	7:A:706:HOH:O	2.46	0.54
1:D:31:VAL:HG21	1:D:66:ASP:HB3	1.89	0.54
1:F:195:TYR:HD2	7:F:585:HOH:O	1.86	0.54
1:F:3:LEU:HG	1:F:291:ASN:HD21	1.72	0.54
1:C:209:PRO:C	7:C:598:HOH:O	2.46	0.54
1:F:3:LEU:HG	1:F:291:ASN:ND2	2.23	0.54
1:C:316:LYS:HE3	7:C:591:HOH:O	2.07	0.54
1:G:10:ILE:CD1	1:G:33:VAL:HG22	2.35	0.54
7:A:697:HOH:O	1:B:202:LEU:CD2	2.55	0.53
1:D:21:LEU:HD13	1:D:71:ILE:HD13	1.90	0.53
1:C:231:GLN:C	7:C:603:HOH:O	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LEU:O	1:D:178[B]:ILE:HG23	2.08	0.53
1:G:147:GLN:N	7:G:802:HOH:O	2.40	0.53
3:G:401:EPE:H71	7:G:808:HOH:O	2.01	0.53
1:A:246:MSE:HG2	7:A:470:HOH:O	2.08	0.53
1:A:5:ALA:HB1	1:A:71:ILE:HD13	1.91	0.53
1:F:87:LEU:O	1:F:116:ASN:ND2	2.40	0.53
1:G:220:ILE:CG2	7:G:785:HOH:O	2.56	0.53
1:A:160:THR:H	1:A:229:ASN:HD21	1.57	0.53
1:B:76:ASN:ND2	2:B:400:NAD:O3D	2.42	0.53
1:F:4:LYS:HG2	1:F:31:VAL:HG11	1.90	0.53
1:A:220:ILE:HD11	7:A:685:HOH:O	2.08	0.52
1:H:333:ASP:HA	1:H:336:LYS:HD2	1.90	0.52
1:C:210:GLN:HB3	7:C:601:HOH:O	2.09	0.52
1:A:119:ARG:HG2	7:A:689:HOH:O	2.10	0.52
1:D:304:GLY:N	7:D:637:HOH:O	2.41	0.52
1:H:13:ILE:HD11	1:H:17:HIS:CE1	2.44	0.52
1:D:235:ASP:OD2	1:D:237:HIS:HE1	1.92	0.52
1:D:301:SER:O	7:D:608:HOH:O	2.19	0.52
1:F:214:MSE:HE1	1:F:310:THR:CG2	2.39	0.52
1:H:118:LYS:O	1:H:120:MSE:HG3	2.10	0.52
1:E:180:VAL:HG11	7:E:769:HOH:O	2.08	0.52
1:A:107:GLN:NE2	7:A:705:HOH:O	2.43	0.52
1:D:314:CYS:CB	7:D:628:HOH:O	2.51	0.52
1:D:315:VAL:HG21	7:D:622:HOH:O	2.09	0.52
1:A:289:ARG:NE	7:A:445:HOH:O	2.28	0.52
1:F:126:MSE:H	1:F:126:MSE:SE	2.43	0.52
1:B:157:ASN:HB3	1:B:228:VAL:HA	1.91	0.52
1:F:12[C]:MSE:SE	1:F:12[C]:MSE:C	2.98	0.52
1:H:13:ILE:O	1:H:13:ILE:HD12	2.09	0.52
1:G:126:MSE:HG3	7:G:780:HOH:O	2.10	0.51
1:G:231:GLN:C	7:G:811:HOH:O	2.47	0.51
1:A:10:ILE:HG13	1:A:33:VAL:CG1	2.41	0.51
1:G:147:GLN:CB	7:G:802:HOH:O	2.45	0.51
1:A:33:VAL:CG1	1:A:41:ALA:HB1	2.40	0.51
1:B:61:LEU:HD23	1:B:61:LEU:C	2.31	0.51
1:G:137:LYS:HB2	7:G:798:HOH:O	2.09	0.51
1:G:210:GLN:NE2	1:G:318:GLN:HE21	1.96	0.51
1:D:294:LEU:HB3	1:D:295:PRO:HD2	1.93	0.51
1:G:3:LEU:HG	1:G:291:ASN:ND2	2.26	0.51
1:B:57:ASP:OD2	1:B:59:HIS:CD2	2.63	0.51
1:C:174:LEU:HD23	1:C:177:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:VAL:HG11	7:D:622:HOH:O	2.09	0.51
1:G:147:GLN:CA	7:G:802:HOH:O	2.58	0.51
1:H:225:GLU:CB	7:H:658:HOH:O	2.29	0.51
1:C:97:LYS:HZ3	1:C:176:HIS:CE1	2.27	0.51
1:D:311:ALA:CA	7:D:628:HOH:O	2.34	0.51
1:G:155:HIS:NE2	7:G:808:HOH:O	2.33	0.51
1:A:214:MSE:HE1	1:A:310:THR:HG22	1.90	0.50
1:C:233:GLY:N	7:C:603:HOH:O	2.41	0.50
1:G:137:LYS:HB3	7:G:798:HOH:O	2.09	0.50
1:H:199:GLN:HE22	1:H:208:ASP:H	1.60	0.50
1:B:172:GLU:OE1	3:B:401:EPE:H31	2.11	0.50
1:H:127:ARG:NH1	7:H:670:HOH:O	2.44	0.50
1:A:12[B]:MSE:HE3	1:A:272:LYS:HZ3	1.73	0.50
1:C:158:ALA:CA	7:C:603:HOH:O	2.24	0.50
1:A:18:LEU:HD11	1:A:50:ILE:HD13	1.94	0.50
1:A:314:CYS:CB	7:A:676:HOH:O	2.60	0.50
1:D:76:ASN:ND2	2:D:400:NAD:O3D	2.44	0.50
1:H:153:GLY:CA	7:H:669:HOH:O	2.56	0.50
7:A:697:HOH:O	1:B:202:LEU:CG	2.51	0.50
1:C:107:GLN:NE2	1:C:305:TYR:HE2	2.09	0.50
1:D:241:THR:CB	7:D:623:HOH:O	2.27	0.50
1:G:183:TRP:HH2	7:G:798:HOH:O	1.90	0.50
1:D:10:ILE:HD11	1:D:33:VAL:HG22	1.93	0.50
1:E:118:LYS:O	1:E:120:MSE:HG3	2.12	0.50
1:F:224:VAL:CG1	7:F:607:HOH:O	2.57	0.50
5:G:402:EDO:C2	7:G:779:HOH:O	2.22	0.49
1:B:19:ARG:HD3	7:B:625:HOH:O	2.12	0.49
1:B:241:THR:C	7:B:635:HOH:O	2.49	0.49
1:C:119:ARG:HD2	1:C:334:PHE:O	2.12	0.49
1:F:285:ASP:OD1	1:F:289:ARG:NH1	2.45	0.49
1:F:331[A]:LYS:N	1:F:331[A]:LYS:HE3	2.21	0.49
1:D:315:VAL:CG1	7:D:622:HOH:O	2.60	0.49
1:D:257:VAL:HB	5:D:402:EDO:H11	1.93	0.49
1:E:257:VAL:HB	5:E:402:EDO:H22	1.95	0.49
1:D:33:VAL:CG1	1:D:41:ALA:HB1	2.34	0.49
1:F:232:TYR:HE2	7:F:580:HOH:O	1.93	0.49
1:A:199:GLN:NE2	1:A:207:ARG:HA	2.25	0.49
1:B:126:MSE:SE	1:B:126:MSE:H	2.46	0.49
2:C:400:NAD:C3D	7:C:614:HOH:O	2.52	0.49
1:D:11:GLY:HA3	2:D:400:NAD:O5B	2.12	0.49
1:D:315:VAL:CG2	7:D:622:HOH:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:CD1	7:B:621:HOH:O	2.55	0.49
1:E:131:LYS:HE2	7:E:765:HOH:O	2.12	0.49
1:F:155:HIS:CE1	7:F:434:HOH:O	2.65	0.49
1:E:151:VAL:HB	7:E:795:HOH:O	2.13	0.49
1:F:93:VAL:HB	1:F:121:VAL:HG22	1.95	0.49
1:A:152:HIS:CD2	7:B:526:HOH:O	2.66	0.49
1:A:254:SER:HB3	1:A:265:THR:HB	1.94	0.49
1:D:178[B]:ILE:HD13	1:D:310:THR:CB	2.36	0.49
1:G:127:ARG:CD	7:G:812:HOH:O	2.52	0.49
1:G:322:ASN:OD1	7:G:762:HOH:O	2.20	0.49
1:G:97:LYS:NZ	1:G:176:HIS:NE2	2.56	0.48
1:H:16:ASP:HB3	7:H:637:HOH:O	2.13	0.48
1:H:327[B]:GLU:HG3	1:H:327[B]:GLU:O	2.12	0.48
1:B:184:LEU:CA	7:B:624:HOH:O	2.21	0.48
1:B:144:GLU:OE2	1:C:259[A]:LYS:HE2	2.13	0.48
1:B:289:ARG:HH11	1:B:289:ARG:CG	2.26	0.48
1:C:150:MSE:HE1	1:D:210:GLN:C	2.33	0.48
1:E:333:ASP:HA	1:E:336:LYS:HD2	1.94	0.48
1:E:97:LYS:C	1:E:97:LYS:HD2	2.33	0.48
1:F:190:LYS:HG3	1:F:191:THR:HG23	1.95	0.48
1:G:71:ILE:HG13	1:G:94:PHE:HB3	1.95	0.48
1:D:21:LEU:CD1	1:D:71:ILE:HD13	2.43	0.48
1:B:237:HIS:HD2	7:B:510:HOH:O	1.95	0.48
1:F:33:VAL:HG11	1:F:45:LEU:HD21	1.95	0.48
1:C:174:LEU:CD2	1:C:174:LEU:O	2.60	0.48
1:D:37:VAL:HB	1:D:40:ARG:CG	2.34	0.48
1:F:181:MSE:CE	7:F:586:HOH:O	2.57	0.48
1:F:200:SER:CB	7:F:620:HOH:O	2.61	0.48
1:G:90:ASN:OD1	1:G:116:ASN:OD1	2.32	0.48
1:A:12[B]:MSE:C	1:A:12[B]:MSE:SE	3.02	0.48
1:A:190:LYS:HG3	1:A:191:THR:HG23	1.95	0.48
1:E:57:ASP:OD1	1:E:59:HIS:CD2	2.66	0.48
1:G:306:LEU:HD23	1:G:328:LEU:HD22	1.95	0.48
1:G:233:GLY:N	7:G:811:HOH:O	2.46	0.48
1:B:214:MSE:CE	1:B:310:THR:CG2	2.92	0.48
1:C:246:MSE:SE	7:C:585:HOH:O	2.78	0.48
1:F:12[C]:MSE:HE3	1:F:272:LYS:HZ3	1.77	0.48
1:B:12[A]:MSE:HE3	1:B:272:LYS:HZ2	1.79	0.47
1:B:128:ARG:HD2	1:B:299:PRO:HG3	1.95	0.47
1:E:289:ARG:NH1	7:E:715:HOH:O	2.23	0.47
1:A:10:ILE:CG1	1:A:33:VAL:HG13	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HD22	1:A:50:ILE:HG12	1.95	0.47
1:B:47:LYS:HD3	1:B:48:TYR:CZ	2.50	0.47
1:F:36:ILE:HG12	2:F:400:NAD:C4A	2.44	0.47
1:A:99:LEU:HD22	7:A:690:HOH:O	2.07	0.47
1:B:333:ASP:HA	1:B:336:LYS:HG3	1.95	0.47
1:C:190:LYS:HE3	7:C:583:HOH:O	2.15	0.47
1:G:57:ASP:HB2	1:G:60:ASP:OD2	2.15	0.47
1:E:199:GLN:HE22	1:E:208:ASP:H	1.61	0.47
1:E:246:MSE:CG	7:E:784:HOH:O	2.45	0.47
1:F:302:TRP:O	1:F:306:LEU:HG	2.14	0.47
1:H:170:ILE:HG12	7:H:647:HOH:O	2.14	0.47
1:F:177:GLU:HA	1:F:180:VAL:HG12	1.96	0.47
1:C:74:ALA:CA	7:C:618:HOH:O	2.60	0.47
1:H:197:PRO:CD	7:H:665:HOH:O	2.42	0.47
7:A:702:HOH:O	1:C:263:TYR:N	2.48	0.47
1:C:210:GLN:N	7:C:598:HOH:O	2.48	0.47
1:E:127:ARG:NH1	7:E:769:HOH:O	2.46	0.47
1:G:127:ARG:HD3	1:G:133:TYR:CE2	2.50	0.47
1:D:171:TYR:CZ	1:D:315:VAL:HG21	2.50	0.47
1:D:310:THR:O	7:D:628:HOH:O	2.21	0.47
1:E:193[B]:LYS:HE3	1:E:322:ASN:O	2.14	0.47
1:F:147:GLN:CG	7:F:616:HOH:O	2.31	0.47
1:F:135[B]:GLN:NE2	7:F:582:HOH:O	2.46	0.46
1:H:171:TYR:CE2	1:H:315:VAL:HG21	2.50	0.46
1:C:118:LYS:O	1:C:120:MSE:HG3	2.15	0.46
1:G:214:MSE:HE1	1:G:310:THR:HG21	1.98	0.46
1:B:126:MSE:HE2	7:B:638:HOH:O	2.13	0.46
1:G:214:MSE:HB3	1:G:214:MSE:HE2	1.85	0.46
1:H:10:ILE:CD1	1:H:33:VAL:HG22	2.44	0.46
1:C:126:MSE:H	1:C:126:MSE:SE	2.48	0.46
5:D:402:EDO:H12	7:D:647:HOH:O	2.15	0.46
1:H:223:VAL:HG13	7:H:635:HOH:O	2.16	0.46
1:F:82:VAL:CG2	7:F:595:HOH:O	2.64	0.46
1:C:315:VAL:CG2	7:C:612:HOH:O	2.64	0.46
1:C:80:ALA:O	1:C:84:VAL:HG23	2.16	0.46
1:A:302:TRP:O	1:A:306:LEU:HG	2.16	0.46
1:C:322:ASN:OD1	7:C:519:HOH:O	2.21	0.46
1:E:5:ALA:HB1	1:E:71:ILE:HD13	1.96	0.46
1:A:128:ARG:HB2	7:A:569:HOH:O	2.16	0.46
1:G:6:GLY:HA2	1:G:32:ALA:O	2.16	0.46
1:B:156:TYR:HA	1:B:227:PHE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ILE:CD1	1:D:33:VAL:HG22	2.46	0.45
1:H:129:TYR:CD1	1:H:282:GLU:HB3	2.51	0.45
1:A:174:LEU:HD22	1:A:177:GLU:HB2	1.99	0.45
1:A:299:PRO:CA	7:A:719:HOH:O	2.15	0.45
1:E:306:LEU:HD23	1:E:328:LEU:HD22	1.98	0.45
1:H:294:LEU:HB3	1:H:295:PRO:HD2	1.99	0.45
1:C:214:MSE:HE1	1:C:310:THR:HG21	1.98	0.45
1:E:127:ARG:HD3	1:E:133:TYR:CE2	2.52	0.45
1:A:17:HIS:HA	1:A:20:ARG:HG3	1.99	0.45
1:C:12:MSE:O	1:C:12:MSE:HE2	2.16	0.45
1:C:197:PRO:CD	7:C:598:HOH:O	2.65	0.45
1:E:209:PRO:HD3	1:F:149:LEU:HD13	1.99	0.45
1:E:225:GLU:C	7:E:771:HOH:O	2.54	0.45
1:F:212:VAL:HG22	7:F:627:HOH:O	2.09	0.45
1:B:302:TRP:HH2	1:B:329:PRO:HG2	1.80	0.45
1:G:126:MSE:HE3	7:G:780:HOH:O	2.15	0.45
1:H:138:ASN:ND2	7:H:571:HOH:O	2.49	0.45
1:A:265:THR:O	7:A:702:HOH:O	2.21	0.44
1:B:97:LYS:O	1:B:97:LYS:HD3	2.17	0.44
1:D:175:ILE:HD11	1:D:307:ALA:HB1	1.98	0.44
1:G:155:HIS:CD2	7:G:808:HOH:O	2.70	0.44
1:G:197:PRO:HG2	7:G:710:HOH:O	2.17	0.44
1:C:137:LYS:NZ	7:C:599:HOH:O	2.50	0.44
1:C:209:PRO:CB	7:C:598:HOH:O	2.65	0.44
1:G:59:HIS:CD2	7:G:667:HOH:O	2.70	0.44
1:H:137:LYS:HE2	1:H:183:TRP:O	2.17	0.44
1:B:172:GLU:N	7:B:627:HOH:O	2.49	0.44
1:C:305:TYR:O	1:C:309:VAL:HG23	2.17	0.44
1:F:162:PRO:HA	1:F:205:THR:HG21	1.99	0.44
1:H:3:LEU:CD1	1:H:290:LEU:HB3	2.48	0.44
1:E:171:TYR:CE2	1:E:315:VAL:HG21	2.53	0.44
1:E:265:THR:HA	5:E:402:EDO:H12	2.00	0.44
7:B:642:HOH:O	1:C:139:ILE:HD11	2.18	0.44
1:F:62:ILE:O	1:F:91:LYS:HE3	2.18	0.44
1:B:37:VAL:O	1:B:40:ARG:HB2	2.18	0.44
1:D:165[B]:LYS:HD2	7:D:610:HOH:O	2.16	0.44
1:D:6:GLY:HA3	1:D:61:LEU:HD21	1.99	0.44
1:F:12[C]:MSE:HE2	1:F:16:ASP:OD2	2.18	0.44
1:H:246:MSE:SE	7:H:432:HOH:O	2.86	0.44
1:C:57:ASP:OD2	1:C:59:HIS:HB2	2.18	0.44
1:D:165[B]:LYS:HE2	1:D:165[B]:LYS:HB3	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LEU:HD12	1:D:177:GLU:HB2	2.00	0.44
1:G:158:ALA:HB3	7:G:770:HOH:O	2.18	0.44
1:G:235:ASP:OD2	1:G:237:HIS:HE1	2.01	0.44
1:H:127:ARG:CB	7:H:639:HOH:O	2.14	0.44
1:H:180:VAL:CG1	7:H:670:HOH:O	2.66	0.44
1:B:189:TYR:CG	1:B:214:MSE:HE2	2.54	0.43
1:E:32:ALA:HA	1:E:53:LYS:O	2.17	0.43
1:E:61:LEU:C	1:E:61:LEU:HD23	2.38	0.43
7:E:634:HOH:O	1:F:152:HIS:HD2	1.73	0.43
1:F:184:LEU:CA	7:F:613:HOH:O	2.30	0.43
1:A:241:THR:CB	7:A:692:HOH:O	2.25	0.43
1:C:289:ARG:HD3	7:C:592:HOH:O	2.18	0.43
1:F:76:ASN:ND2	2:F:400:NAD:O3D	2.51	0.43
1:F:34:CYS:HA	1:F:55:TYR:O	2.19	0.43
1:F:44:ALA:O	1:F:48:TYR:HD2	2.02	0.43
1:A:65:LYS:N	1:A:65:LYS:HD2	2.33	0.43
1:C:137:LYS:HD2	1:C:183:TRP:CZ2	2.53	0.43
1:C:6:GLY:HA3	1:C:61:LEU:HD21	2.00	0.43
1:A:180:VAL:CG1	7:A:711:HOH:O	2.67	0.43
1:D:165[B]:LYS:NZ	7:D:611:HOH:O	2.47	0.43
1:D:61:LEU:HD23	1:D:61:LEU:C	2.39	0.43
1:E:222:ILE:HG12	7:E:795:HOH:O	2.12	0.43
1:F:192:VAL:HG11	1:F:214:MSE:HE3	2.00	0.43
1:G:64:ASP:OD1	1:G:66:ASP:HB2	2.19	0.43
1:D:222:ILE:CB	7:D:643:HOH:O	2.55	0.43
1:C:162:PRO:HA	1:C:205:THR:HG21	2.01	0.43
1:E:151:VAL:HG23	7:E:795:HOH:O	2.18	0.43
1:A:13:ILE:HD11	1:A:17:HIS:CE1	2.54	0.42
1:C:180:VAL:HB	7:C:615:HOH:O	2.19	0.42
1:D:237:HIS:CD2	7:D:615:HOH:O	2.65	0.42
1:F:193:LYS:C	7:F:585:HOH:O	2.56	0.42
1:A:128:ARG:HD3	1:A:183:TRP:CD1	2.55	0.42
1:E:246:MSE:O	1:H:257:VAL:HA	2.19	0.42
1:G:17:HIS:O	1:G:21:LEU:HG	2.18	0.42
1:A:95:CYS:O	1:A:123:ILE:HA	2.19	0.42
1:B:122:GLN:CD	1:B:298:GLY:HA3	2.40	0.42
1:B:235:ASP:CG	1:B:237:HIS:HE1	2.21	0.42
1:F:255:ALA:CB	7:G:782:HOH:O	2.67	0.42
1:G:214:MSE:HE1	1:G:310:THR:CG2	2.50	0.42
1:G:3:LEU:HG	1:G:291:ASN:HD21	1.85	0.42
1:H:174:LEU:HD12	1:H:177:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:304:GLY:N	7:H:654:HOH:O	2.49	0.42
1:A:127:ARG:HD3	1:A:133:TYR:CE2	2.54	0.42
1:D:118:LYS:O	1:D:120:MSE:HG3	2.18	0.42
1:D:127:ARG:HG3	7:D:437:HOH:O	2.18	0.42
1:E:259:LYS:O	1:E:260:ALA:C	2.55	0.42
1:E:77:GLU:CD	7:E:783:HOH:O	2.56	0.42
1:F:290:LEU:HD11	1:F:296:PRO:HD3	2.00	0.42
1:D:259:LYS:O	1:D:260:ALA:C	2.58	0.42
1:G:134:VAL:CA	7:G:798:HOH:O	2.50	0.42
1:B:289:ARG:CG	1:B:289:ARG:NH1	2.82	0.42
1:B:77:GLU:CD	1:B:77:GLU:H	2.23	0.42
1:E:17:HIS:ND1	1:E:20:ARG:NH1	2.68	0.42
1:F:33:VAL:HG21	1:F:41:ALA:HB1	1.93	0.42
1:A:8:VAL:C	7:A:723:HOH:O	2.58	0.42
1:C:279:TYR:OH	2:C:400:NAD:N7N	2.53	0.42
1:E:6:GLY:HA3	1:E:61:LEU:HD21	2.02	0.42
1:A:174:LEU:HD13	1:A:178:ILE:HD11	2.02	0.42
1:A:199:GLN:HE22	1:A:208:ASP:H	1.67	0.42
1:C:197:PRO:HD2	7:C:598:HOH:O	2.19	0.42
1:E:3:LEU:HD11	1:E:290:LEU:HB3	2.02	0.42
7:E:768:HOH:O	1:G:262:LYS:HB3	2.20	0.42
1:C:211:LEU:HD23	1:C:225:GLU:HG2	2.02	0.42
1:H:95:CYS:O	1:H:123:ILE:HA	2.19	0.42
1:C:221:ASN:HA	7:C:586:HOH:O	2.19	0.41
1:G:2:THR:HG22	1:G:27:GLY:HA2	2.02	0.41
1:A:32:ALA:CB	7:A:684:HOH:O	2.67	0.41
1:C:210:GLN:HE22	1:C:318:GLN:NE2	2.05	0.41
1:H:144:GLU:HG3	1:H:144:GLU:O	2.20	0.41
1:A:175:ILE:HD11	1:A:307:ALA:HB1	2.02	0.41
1:B:315:VAL:O	1:B:319:GLU:HG3	2.19	0.41
1:F:107:GLN:O	1:F:111:GLU:HG3	2.20	0.41
1:F:193:LYS:NZ	1:F:321:GLY:O	2.53	0.41
1:C:32:ALA:HB3	1:C:61:LEU:HD22	2.03	0.41
1:E:267:ILE:HG23	7:E:758:HOH:O	2.07	0.41
1:A:178:ILE:CD1	7:A:680:HOH:O	2.40	0.41
1:B:177:GLU:O	1:B:181:MSE:HG2	2.20	0.41
1:C:197:PRO:CG	7:C:598:HOH:O	2.62	0.41
1:C:235:ASP:OD2	1:C:237:HIS:HE1	2.03	0.41
1:F:175:ILE:HD11	1:F:307:ALA:HB1	2.03	0.41
1:G:238:CYS:HB2	7:G:791:HOH:O	2.21	0.41
1:H:126:MSE:SE	1:H:126:MSE:H	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:ILE:HG21	1:H:314:CYS:HB2	2.02	0.41
1:A:160:THR:HG22	3:A:401:EPE:H91	2.01	0.41
1:A:35:ASP:OD1	1:A:36:ILE:N	2.53	0.41
1:B:172:GLU:OE2	3:B:401:EPE:H51	2.21	0.41
1:C:126:MSE:CE	2:C:400:NAD:H72N	2.34	0.41
1:E:126:MSE:SE	1:E:126:MSE:H	2.53	0.41
7:E:634:HOH:O	1:F:223:VAL:HG11	2.20	0.41
1:A:290:LEU:HA	1:A:290:LEU:HD12	1.91	0.41
1:B:184:LEU:HD13	7:B:620:HOH:O	2.20	0.41
1:F:200:SER:HB3	7:F:620:HOH:O	2.19	0.41
1:F:129:TYR:CD1	1:F:282:GLU:HB3	2.55	0.41
1:G:236:ILE:HG22	7:G:791:HOH:O	2.21	0.41
1:A:192:VAL:CG1	7:A:709:HOH:O	2.47	0.41
1:A:220:ILE:HG13	7:A:679:HOH:O	2.20	0.41
1:B:144:GLU:CG	1:C:259[A]:LYS:HE2	2.45	0.41
1:E:21:LEU:HD23	1:E:21:LEU:HA	1.87	0.41
1:F:189:TYR:CG	1:F:214:MSE:HE2	2.55	0.41
1:B:263:TYR:N	7:D:663:HOH:O	2.54	0.41
1:F:171:TYR:HA	7:F:614:HOH:O	2.20	0.41
1:G:97:LYS:HE2	1:G:176:HIS:NE2	2.36	0.41
1:C:243:GLU:CG	7:C:596:HOH:O	2.66	0.41
1:C:271:TRP:CD2	3:C:401:EPE:H52	2.56	0.41
1:D:178[B]:ILE:HA	7:D:614:HOH:O	2.20	0.41
1:F:289:ARG:NE	7:F:474:HOH:O	2.53	0.41
1:F:144:GLU:HG2	1:G:259:LYS:HE2	2.03	0.41
1:C:61:LEU:C	1:C:61:LEU:CD1	2.88	0.40
1:D:61:LEU:HD22	7:D:641:HOH:O	2.20	0.40
1:A:259:LYS:O	1:A:260:ALA:C	2.60	0.40
1:B:162:PRO:HA	1:B:205:THR:HG21	2.02	0.40
1:D:61:LEU:CD2	7:D:641:HOH:O	2.70	0.40
1:F:273:GLN:HG3	7:F:577:HOH:O	2.20	0.40
1:B:2:THR:HG23	1:B:2:THR:O	2.22	0.40
1:B:40:ARG:CD	7:B:626:HOH:O	2.69	0.40
1:D:138:ASN:ND2	7:D:516:HOH:O	2.55	0.40
1:E:171:TYR:CZ	1:E:315:VAL:HG21	2.56	0.40
1:F:226:VAL:C	7:F:591:HOH:O	2.60	0.40
1:G:59:HIS:CB	7:G:667:HOH:O	2.62	0.40
1:A:32:ALA:HA	1:A:53:LYS:O	2.22	0.40
1:B:184:LEU:HD13	7:B:624:HOH:O	2.18	0.40
1:D:328:LEU:CD1	7:D:491:HOH:O	2.42	0.40
1:F:25:VAL:CG1	7:F:629:HOH:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:TYR:HE1	7:G:814:HOH:O	2.04	0.40
1:G:3:LEU:CD1	1:G:290:LEU:HB3	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:607:HOH:O	7:E:703:HOH:O[1_455]	2.18	0.02

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	338/357 (95%)	328 (97%)	10 (3%)	0	100	100
1	B	335/357 (94%)	322 (96%)	13 (4%)	0	100	100
1	C	334/357 (94%)	322 (96%)	12 (4%)	0	100	100
1	D	338/357 (95%)	326 (96%)	12 (4%)	0	100	100
1	E	337/357 (94%)	325 (96%)	12 (4%)	0	100	100
1	F	337/357 (94%)	321 (95%)	16 (5%)	0	100	100
1	G	334/357 (94%)	319 (96%)	15 (4%)	0	100	100
1	H	336/357 (94%)	324 (96%)	12 (4%)	0	100	100
All	All	2689/2856 (94%)	2587 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	284/290 (98%)	271 (95%)	13 (5%)	27 23
1	B	282/290 (97%)	256 (91%)	26 (9%)	9 5
1	C	281/290 (97%)	262 (93%)	19 (7%)	16 10
1	D	284/290 (98%)	266 (94%)	18 (6%)	18 13
1	E	283/290 (98%)	270 (95%)	13 (5%)	27 23
1	F	284/290 (98%)	267 (94%)	17 (6%)	19 14
1	G	281/290 (97%)	269 (96%)	12 (4%)	29 27
1	H	282/290 (97%)	269 (95%)	13 (5%)	27 23
All	All	2261/2320 (98%)	2130 (94%)	131 (6%)	20 15

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	50	ILE
1	A	97	LYS
1	A	119	ARG
1	A	126	MSE
1	A	174	LEU
1	A	180	VAL
1	A	182	HIS
1	A	184	LEU
1	A	207	ARG
1	A	227	PHE
1	A	268	LEU
1	A	290	LEU
1	B	3	LEU
1	B	12[A]	MSE
1	B	12[B]	MSE
1	B	13	ILE
1	B	29	GLU
1	B	31	VAL
1	B	53	LYS
1	B	54	ASP
1	B	64	ASP
1	B	65	LYS

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Mol	Chain	Res	Type
1	B	68	GLU
1	B	73	THR
1	B	97	LYS
1	B	118	LYS
1	B	126	MSE
1	B	180	VAL
1	B	184	LEU
1	B	206	LEU
1	B	221	ASN
1	B	268	LEU
1	B	276	ILE
1	B	289	ARG
1	B	290	LEU
1	B	312	ASP
1	B	330	SER
1	B	336	LYS
1	C	2	THR
1	C	12	MSE
1	C	13	ILE
1	C	15	SER
1	C	54	ASP
1	C	61	LEU
1	C	66	ASP
1	C	97	LYS
1	C	107	GLN
1	C	126	MSE
1	C	130	ASP
1	C	174	LEU
1	C	180	VAL
1	C	182	HIS
1	C	184	LEU
1	C	206	LEU
1	C	227	PHE
1	C	290	LEU
1	C	312	ASP
1	D	2	THR
1	D	4	LYS
1	D	33	VAL
1	D	36	ILE
1	D	51	GLU
1	D	53	LYS
1	D	97	LYS

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Mol	Chain	Res	Type
1	D	119	ARG
1	D	126	MSE
1	D	180	VAL
1	D	184	LEU
1	D	206	LEU
1	D	227	PHE
1	D	268	LEU
1	D	276	ILE
1	D	290	LEU
1	D	312	ASP
1	D	328	LEU
1	E	12	MSE
1	E	65	LYS
1	E	73	THR
1	E	97	LYS
1	E	107	GLN
1	E	126	MSE
1	E	172	GLU
1	E	180	VAL
1	E	184	LEU
1	E	221	ASN
1	E	227	PHE
1	E	276	ILE
1	E	290	LEU
1	F	2	THR
1	F	4	LYS
1	F	15	SER
1	F	33	VAL
1	F	66	ASP
1	F	69	VAL
1	F	97	LYS
1	F	116	ASN
1	F	126	MSE
1	F	182	HIS
1	F	184	LEU
1	F	206	LEU
1	F	221	ASN
1	F	227	PHE
1	F	289	ARG
1	F	331[A]	LYS
1	F	331[B]	LYS
1	G	13	ILE

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Mol	Chain	Res	Type
1	G	33	VAL
1	G	66	ASP
1	G	97	LYS
1	G	119	ARG
1	G	126	MSE
1	G	184	LEU
1	G	206	LEU
1	G	227	PHE
1	G	268	LEU
1	G	276	ILE
1	G	312	ASP
1	H	12	MSE
1	H	13	ILE
1	H	33	VAL
1	H	36	ILE
1	H	66	ASP
1	H	97	LYS
1	H	126	MSE
1	H	144	GLU
1	H	180	VAL
1	H	182	HIS
1	H	184	LEU
1	H	227	PHE
1	H	290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	76	ASN
1	A	88	ASN
1	A	138	ASN
1	A	199	GLN
1	A	210	GLN
1	A	229	ASN
1	A	231	GLN
1	B	23	ASN
1	B	59	HIS
1	B	76	ASN
1	B	88	ASN
1	B	114	GLN
1	B	138	ASN

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	221	ASN
1	B	231	GLN
1	B	237	HIS
1	C	76	ASN
1	C	88	ASN
1	C	107	GLN
1	C	114	GLN
1	C	138	ASN
1	C	199	GLN
1	C	210	GLN
1	C	221	ASN
1	C	231	GLN
1	C	237	HIS
1	C	291	ASN
1	C	322	ASN
1	D	76	ASN
1	D	88	ASN
1	D	138	ASN
1	D	231	GLN
1	D	237	HIS
1	E	59	HIS
1	E	76	ASN
1	E	88	ASN
1	E	107	GLN
1	E	138	ASN
1	E	199	GLN
1	E	210	GLN
1	E	221	ASN
1	E	237	HIS
1	F	76	ASN
1	F	88	ASN
1	F	147	GLN
1	F	221	ASN
1	F	231	GLN
1	F	291	ASN
1	G	42	GLN
1	G	59	HIS
1	G	76	ASN
1	G	88	ASN
1	G	138	ASN
1	G	210	GLN

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Mol	Chain	Res	Type
1	G	237	HIS
1	G	291	ASN
1	G	322	ASN
1	H	76	ASN
1	H	88	ASN
1	H	138	ASN
1	H	199	GLN
1	H	210	GLN
1	H	221	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EPE	C	401	-	15,15,15	1.11	1 (6%)	18,20,20	2.43	6 (33%)
2	NAD	E	400	-	42,48,48	1.86	4 (9%)	50,73,73	1.47	4 (8%)
2	NAD	B	400	-	42,48,48	1.86	6 (14%)	50,73,73	1.25	3 (6%)
3	EPE	D	401	-	15,15,15	1.02	1 (6%)	18,20,20	2.08	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	H	402	-	3,3,3	0.45	0	2,2,2	0.87	0
3	EPE	B	401	-	15,15,15	1.20	1 (6%)	18,20,20	2.00	6 (33%)
4	ACY	A	402	-	1,3,3	0.48	0	0,3,3	0.00	-
2	NAD	H	400	-	42,48,48	1.75	3 (7%)	50,73,73	1.31	4 (8%)
5	EDO	D	402	-	3,3,3	0.28	0	2,2,2	0.79	0
2	NAD	D	400	-	42,48,48	1.80	3 (7%)	50,73,73	1.32	6 (12%)
5	EDO	E	403	-	3,3,3	0.25	0	2,2,2	1.00	0
2	NAD	F	400	-	42,48,48	1.79	4 (9%)	50,73,73	1.22	2 (4%)
3	EPE	G	401	-	15,15,15	1.08	1 (6%)	18,20,20	2.24	9 (50%)
3	EPE	H	401	-	15,15,15	1.12	1 (6%)	18,20,20	2.08	6 (33%)
3	EPE	E	401	-	15,15,15	1.11	1 (6%)	18,20,20	3.59	11 (61%)
5	EDO	G	402	-	3,3,3	0.50	0	2,2,2	0.41	0
4	ACY	A	403	-	1,3,3	1.16	0	0,3,3	0.00	-
3	EPE	F	401	-	15,15,15	1.15	1 (6%)	18,20,20	1.82	4 (22%)
3	EPE	A	401	-	15,15,15	0.94	1 (6%)	18,20,20	2.14	5 (27%)
2	NAD	G	400	-	42,48,48	1.73	5 (11%)	50,73,73	1.30	3 (6%)
5	EDO	E	402	-	3,3,3	0.50	0	2,2,2	0.77	0
2	NAD	C	400	-	42,48,48	1.72	3 (7%)	50,73,73	1.27	3 (6%)
2	NAD	A	400	-	42,48,48	1.67	4 (9%)	50,73,73	1.57	7 (14%)

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	H	400	-	-	6/26/62/62	0/5/5/5
5	EDO	E	403	-	-	1/1/1/1	-
3	EPE	D	401	-	-	2/9/19/19	0/1/1/1
2	NAD	D	400	-	-	7/26/62/62	0/5/5/5
3	EPE	G	401	-	-	5/9/19/19	0/1/1/1
2	NAD	G	400	-	-	2/26/62/62	0/5/5/5
3	EPE	F	401	-	-	7/9/19/19	0/1/1/1
3	EPE	A	401	-	-	0/9/19/19	0/1/1/1
2	NAD	E	400	-	-	2/26/62/62	0/5/5/5
5	EDO	D	402	-	-	1/1/1/1	-
3	EPE	E	401	-	-	6/9/19/19	0/1/1/1
3	EPE	C	401	-	-	6/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	G	402	-	-	1/1/1/1	-
5	EDO	H	402	-	-	1/1/1/1	-
3	EPE	H	401	-	-	0/9/19/19	0/1/1/1
2	NAD	F	400	-	-	6/26/62/62	0/5/5/5
2	NAD	B	400	-	-	3/26/62/62	0/5/5/5
2	NAD	C	400	-	-	3/26/62/62	0/5/5/5
5	EDO	E	402	-	-	0/1/1/1	-
2	NAD	A	400	-	-	4/26/62/62	0/5/5/5
3	EPE	B	401	-	-	5/9/19/19	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	NAD	O7N-C7N	9.17	1.41	1.24
2	B	400	NAD	O7N-C7N	9.12	1.41	1.24
2	D	400	NAD	O7N-C7N	8.88	1.41	1.24
2	F	400	NAD	O7N-C7N	8.77	1.40	1.24
2	H	400	NAD	O7N-C7N	8.76	1.40	1.24
2	G	400	NAD	O7N-C7N	8.41	1.40	1.24
2	C	400	NAD	O7N-C7N	8.21	1.39	1.24
2	A	400	NAD	O7N-C7N	8.03	1.39	1.24
2	D	400	NAD	C2A-N3A	4.56	1.39	1.32
3	B	401	EPE	C10-S	4.28	1.83	1.77
2	H	400	NAD	C2A-N3A	4.27	1.39	1.32
2	C	400	NAD	C2A-N3A	4.12	1.38	1.32
2	A	400	NAD	C2A-N3A	4.10	1.38	1.32
2	B	400	NAD	C2A-N3A	4.09	1.38	1.32
2	G	400	NAD	C2A-N3A	4.08	1.38	1.32
2	F	400	NAD	C2A-N3A	3.90	1.38	1.32
3	F	401	EPE	C10-S	3.89	1.83	1.77
3	C	401	EPE	C10-S	3.84	1.83	1.77
3	G	401	EPE	C10-S	3.81	1.82	1.77
3	H	401	EPE	C10-S	3.79	1.82	1.77
2	E	400	NAD	C2A-N3A	3.78	1.38	1.32
3	D	401	EPE	C10-S	3.46	1.82	1.77
3	E	401	EPE	C10-S	3.09	1.81	1.77
3	A	401	EPE	C10-S	2.99	1.81	1.77
2	H	400	NAD	C2A-N1A	2.98	1.39	1.33
2	E	400	NAD	C2A-N1A	2.94	1.39	1.33
2	D	400	NAD	C2A-N1A	2.94	1.39	1.33
2	F	400	NAD	C2N-N1N	2.81	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NAD	O4D-C1D	2.72	1.44	1.41
2	F	400	NAD	C2A-N1A	2.66	1.38	1.33
2	B	400	NAD	C2A-N1A	2.56	1.38	1.33
2	B	400	NAD	C2N-N1N	2.51	1.38	1.35
2	E	400	NAD	C2N-N1N	2.50	1.38	1.35
2	C	400	NAD	C2A-N1A	2.43	1.38	1.33
2	B	400	NAD	O4B-C1B	2.34	1.44	1.41
2	G	400	NAD	C2A-N1A	2.34	1.38	1.33
2	A	400	NAD	C2A-N1A	2.23	1.38	1.33
2	B	400	NAD	C2D-C1D	-2.11	1.50	1.53
2	G	400	NAD	C2N-N1N	2.02	1.37	1.35
2	G	400	NAD	C2D-C1D	-2.01	1.50	1.53

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	401	EPE	O3S-S-C10	8.76	119.94	105.77
3	E	401	EPE	O1S-S-C10	-7.41	97.99	106.92
3	E	401	EPE	C6-N1-C2	6.70	123.91	108.83
2	A	400	NAD	N3A-C2A-N1A	-6.52	118.48	128.68
2	E	400	NAD	N3A-C2A-N1A	-6.40	118.67	128.68
2	B	400	NAD	N3A-C2A-N1A	-6.18	119.02	128.68
2	G	400	NAD	N3A-C2A-N1A	-6.04	119.23	128.68
2	F	400	NAD	N3A-C2A-N1A	-5.88	119.49	128.68
2	H	400	NAD	N3A-C2A-N1A	-5.86	119.52	128.68
2	C	400	NAD	N3A-C2A-N1A	-5.70	119.76	128.68
2	D	400	NAD	N3A-C2A-N1A	-5.59	119.95	128.68
3	C	401	EPE	C5-N4-C3	5.46	121.13	108.83
3	A	401	EPE	O1S-S-C10	5.37	113.39	106.92
3	C	401	EPE	O2S-S-C10	5.33	113.34	106.92
3	B	401	EPE	C5-N4-C3	5.18	120.48	108.83
3	H	401	EPE	C5-N4-C3	4.51	118.99	108.83
3	G	401	EPE	C5-N4-C3	4.39	118.71	108.83
3	D	401	EPE	C5-N4-C3	4.36	118.64	108.83
3	D	401	EPE	O3S-S-C10	4.36	112.82	105.77
3	C	401	EPE	C6-C5-N4	3.97	118.79	110.64
3	A	401	EPE	C5-N4-C3	3.90	117.61	108.83
3	H	401	EPE	O1S-S-C10	3.77	111.45	106.92
3	F	401	EPE	O3S-S-C10	3.34	111.17	105.77
3	E	401	EPE	C5-N4-C3	3.25	116.15	108.83
3	G	401	EPE	C9-N1-C2	-3.23	102.97	111.23
3	F	401	EPE	C7-N4-C5	3.22	119.47	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	EPE	C6-N1-C2	3.20	116.04	108.83
3	G	401	EPE	O3S-S-C10	3.17	110.89	105.77
2	E	400	NAD	C1B-N9A-C4A	-3.17	121.08	126.64
2	A	400	NAD	PN-O3-PA	-3.16	121.97	132.83
3	B	401	EPE	C7-N4-C5	3.06	119.05	111.23
3	F	401	EPE	C5-N4-C3	3.04	115.68	108.83
2	A	400	NAD	C3N-C7N-N7N	3.00	121.35	117.75
3	A	401	EPE	O2S-S-C10	-2.97	103.34	106.92
3	D	401	EPE	O1S-S-C10	-2.95	103.37	106.92
3	H	401	EPE	O2S-S-C10	-2.87	103.46	106.92
3	B	401	EPE	O2S-S-C10	2.87	110.37	106.92
3	F	401	EPE	C6-N1-C2	2.86	115.26	108.83
2	A	400	NAD	O3D-C3D-C4D	-2.82	102.90	111.05
2	G	400	NAD	PN-O3-PA	-2.77	123.31	132.83
3	A	401	EPE	C9-N1-C6	-2.77	104.15	111.23
3	H	401	EPE	C7-N4-C3	2.75	118.27	111.23
2	A	400	NAD	C1B-N9A-C4A	-2.72	121.86	126.64
3	H	401	EPE	C7-N4-C5	2.71	118.17	111.23
3	D	401	EPE	C9-N1-C6	-2.70	104.32	111.23
3	A	401	EPE	C7-N4-C3	2.64	117.97	111.23
3	G	401	EPE	C7-N4-C3	2.62	117.92	111.23
3	G	401	EPE	O1S-S-C10	2.61	110.05	106.92
2	H	400	NAD	PN-O3-PA	-2.58	123.99	132.83
2	H	400	NAD	O2N-PN-O1N	2.55	124.86	112.24
3	E	401	EPE	C3-C2-N1	2.52	115.81	110.64
3	G	401	EPE	O2S-S-C10	-2.51	103.89	106.92
2	C	400	NAD	PN-O3-PA	-2.51	124.20	132.83
3	G	401	EPE	C6-C5-N4	2.51	115.80	110.64
3	G	401	EPE	C6-N1-C2	2.49	114.42	108.83
2	H	400	NAD	C4A-C5A-N7A	-2.46	106.83	109.40
2	G	400	NAD	O3D-C3D-C4D	-2.45	103.96	111.05
2	B	400	NAD	O2N-PN-O1N	2.43	124.28	112.24
3	E	401	EPE	C2-C3-N4	2.42	115.61	110.64
3	B	401	EPE	C6-N1-C2	2.41	114.25	108.83
3	E	401	EPE	O3S-S-O2S	-2.37	105.49	111.27
2	F	400	NAD	O2N-PN-O1N	2.32	123.70	112.24
3	D	401	EPE	C2-C3-N4	2.31	115.39	110.64
3	C	401	EPE	C7-N4-C5	2.30	117.12	111.23
2	E	400	NAD	PN-O3-PA	-2.30	124.93	132.83
2	B	400	NAD	PN-O3-PA	-2.28	125.01	132.83
3	E	401	EPE	C9-N1-C2	2.24	116.95	111.23
2	D	400	NAD	PN-O3-PA	-2.22	125.19	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	401	EPE	C9-N1-C6	-2.22	105.55	111.23
3	E	401	EPE	C6-C5-N4	2.22	115.19	110.64
3	B	401	EPE	C7-N4-C3	2.22	116.90	111.23
3	B	401	EPE	C6-C5-N4	2.18	115.11	110.64
3	C	401	EPE	C9-N1-C2	-2.17	105.68	111.23
3	G	401	EPE	C7-N4-C5	2.16	116.77	111.23
2	C	400	NAD	O2N-PN-O1N	2.16	122.92	112.24
3	E	401	EPE	C7-N4-C3	2.15	116.73	111.23
2	D	400	NAD	O4B-C1B-C2B	-2.12	103.82	106.93
2	A	400	NAD	O5B-C5B-C4B	-2.11	101.73	108.99
3	D	401	EPE	C7-N4-C3	2.09	116.58	111.23
2	A	400	NAD	O4B-C4B-C3B	2.09	109.24	105.11
2	E	400	NAD	O2N-PN-O1N	2.07	122.45	112.24
2	D	400	NAD	O3B-C3B-C4B	-2.06	105.10	111.05
2	D	400	NAD	C4A-C5A-N7A	-2.05	107.26	109.40
3	E	401	EPE	O2S-S-C10	-2.04	104.46	106.92
2	D	400	NAD	O2N-PN-O1N	2.03	122.27	112.24

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	EPE	C10-C9-N1-C6
3	C	401	EPE	S-C10-C9-N1
3	C	401	EPE	C9-C10-S-O2S
2	E	400	NAD	O4D-C1D-N1N-C6N
2	B	400	NAD	O4D-C1D-N1N-C6N
3	B	401	EPE	C10-C9-N1-C6
2	H	400	NAD	O4D-C1D-N1N-C2N
2	H	400	NAD	O4D-C1D-N1N-C6N
2	H	400	NAD	C2D-C1D-N1N-C2N
2	D	400	NAD	O4D-C1D-N1N-C2N
2	D	400	NAD	O4D-C1D-N1N-C6N
2	D	400	NAD	C2D-C1D-N1N-C2N
2	D	400	NAD	C2D-C1D-N1N-C6N
2	F	400	NAD	C5B-O5B-PA-O1A
2	F	400	NAD	O4B-C4B-C5B-O5B
2	F	400	NAD	O4D-C1D-N1N-C6N
3	G	401	EPE	C8-C7-N4-C3
3	E	401	EPE	C9-C10-S-O1S
3	E	401	EPE	C9-C10-S-O2S
3	E	401	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
2	G	400	NAD	O4D-C1D-N1N-C6N
2	C	400	NAD	O4D-C1D-N1N-C6N
2	A	400	NAD	O4D-C1D-N1N-C2N
2	A	400	NAD	O4D-C1D-N1N-C6N
3	B	401	EPE	N4-C7-C8-O8
2	F	400	NAD	C3B-C4B-C5B-O5B
3	C	401	EPE	C9-C10-S-O3S
3	B	401	EPE	C9-C10-S-O3S
3	F	401	EPE	N4-C7-C8-O8
5	D	402	EDO	O1-C1-C2-O2
5	E	403	EDO	O1-C1-C2-O2
5	G	402	EDO	O1-C1-C2-O2
3	D	401	EPE	C9-C10-S-O3S
3	G	401	EPE	C9-C10-S-O3S
3	E	401	EPE	N4-C7-C8-O8
2	B	400	NAD	O4B-C4B-C5B-O5B
3	C	401	EPE	C8-C7-N4-C3
3	F	401	EPE	C8-C7-N4-C5
3	G	401	EPE	C10-C9-N1-C2
3	G	401	EPE	C10-C9-N1-C6
3	E	401	EPE	C10-C9-N1-C6
3	F	401	EPE	C10-C9-N1-C6
2	E	400	NAD	O4B-C4B-C5B-O5B
2	C	400	NAD	O4B-C4B-C5B-O5B
2	D	400	NAD	O4B-C4B-C5B-O5B
2	G	400	NAD	O4B-C4B-C5B-O5B
2	F	400	NAD	C5B-O5B-PA-O2A
3	C	401	EPE	C9-C10-S-O1S
3	B	401	EPE	C9-C10-S-O1S
3	B	401	EPE	C9-C10-S-O2S
3	G	401	EPE	C9-C10-S-O1S
2	H	400	NAD	O4B-C4B-C5B-O5B
3	E	401	EPE	C8-C7-N4-C3
2	A	400	NAD	O4B-C4B-C5B-O5B
3	F	401	EPE	C10-C9-N1-C2
5	H	402	EDO	O1-C1-C2-O2
2	B	400	NAD	C3B-C4B-C5B-O5B
2	D	400	NAD	C3B-C4B-C5B-O5B
3	F	401	EPE	C9-C10-S-O3S
3	F	401	EPE	C8-C7-N4-C3
2	H	400	NAD	C2D-C1D-N1N-C6N
2	F	400	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	A	400	NAD	C2D-C1D-N1N-C2N
2	H	400	NAD	PA-O3-PN-O1N
2	D	400	NAD	PA-O3-PN-O1N
3	D	401	EPE	N4-C7-C8-O8
2	C	400	NAD	C3B-C4B-C5B-O5B
3	F	401	EPE	C9-C10-S-O2S

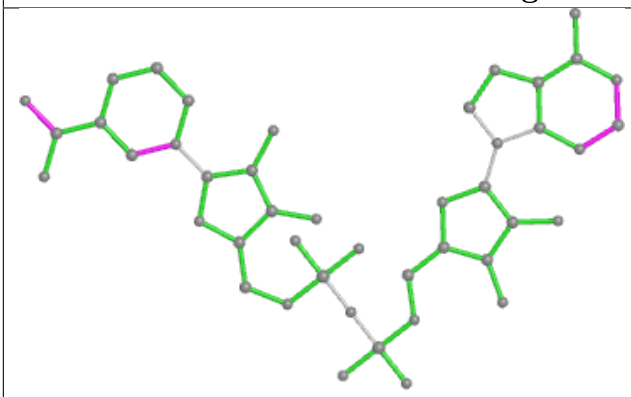
There are no ring outliers.

15 monomers are involved in 31 short contacts:

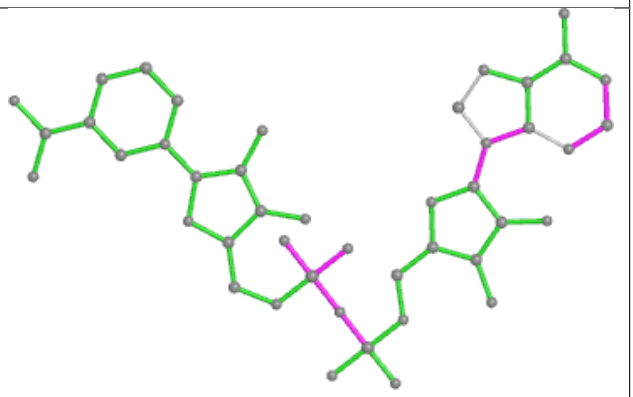
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	EPE	2	0
2	B	400	NAD	1	0
3	B	401	EPE	2	0
4	A	402	ACY	1	0
2	H	400	NAD	1	0
5	D	402	EDO	3	0
2	D	400	NAD	2	0
2	F	400	NAD	2	0
3	G	401	EPE	4	0
3	E	401	EPE	1	0
5	G	402	EDO	3	0
3	A	401	EPE	1	0
5	E	402	EDO	3	0
2	C	400	NAD	4	0
2	A	400	NAD	1	0

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.

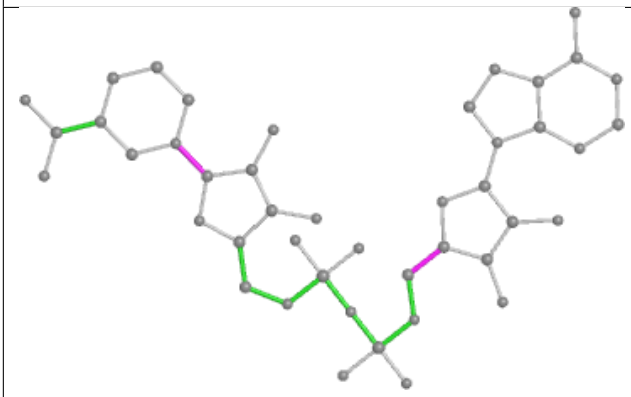
Ligand NAD E 400



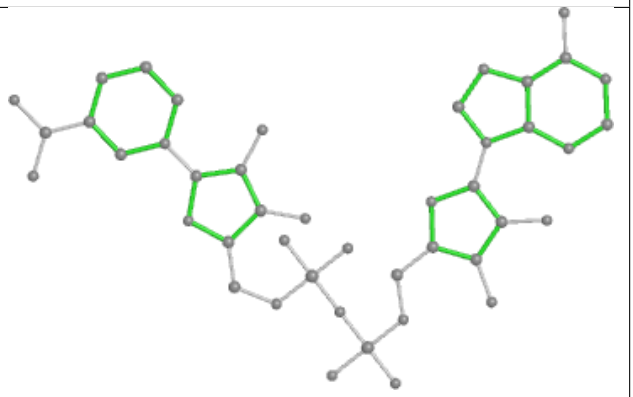
Bond lengths



Bond angles

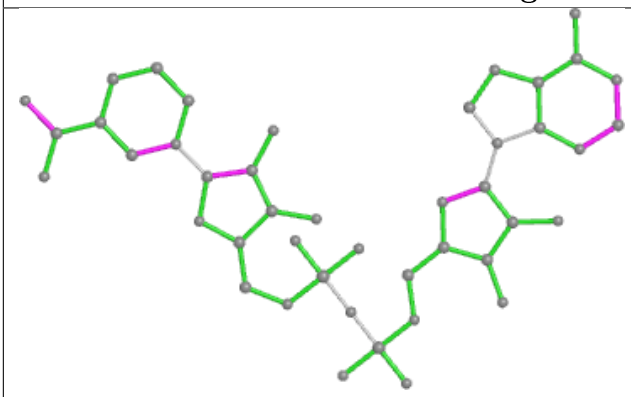


Torsions

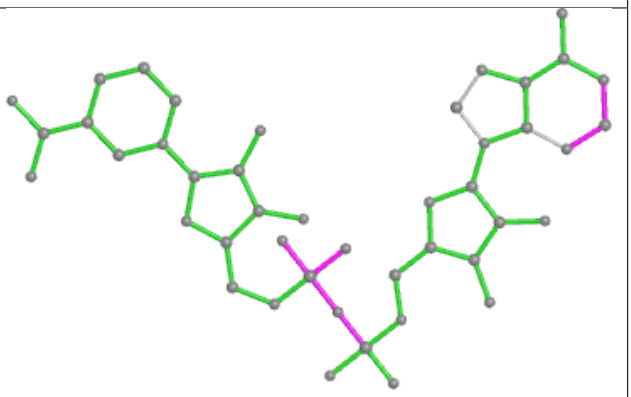


Rings

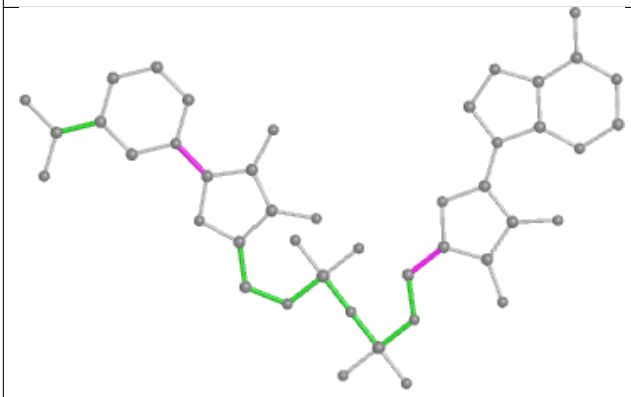
Ligand NAD B 400



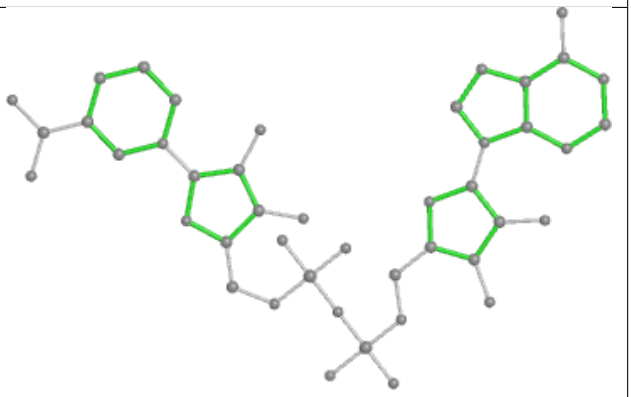
Bond lengths



Bond angles

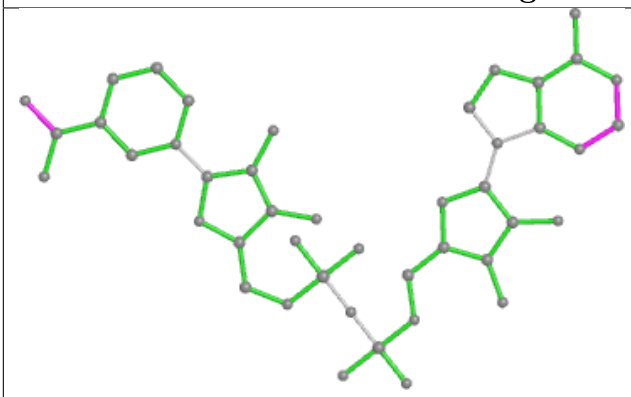


Torsions

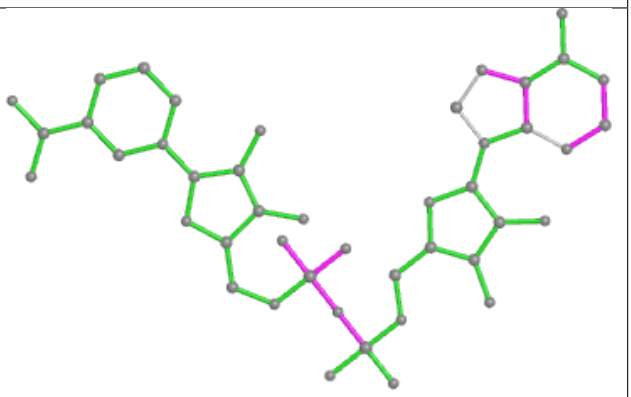


Rings

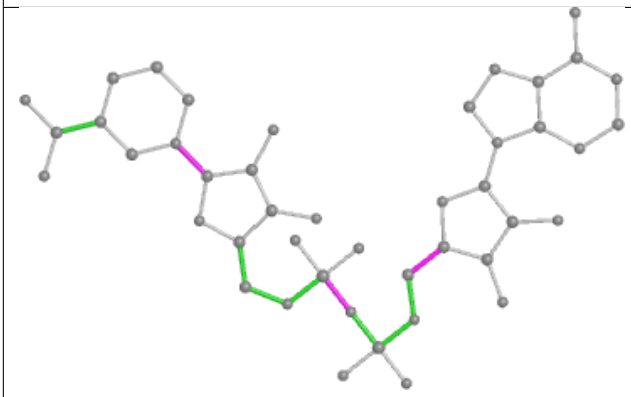
Ligand NAD H 400



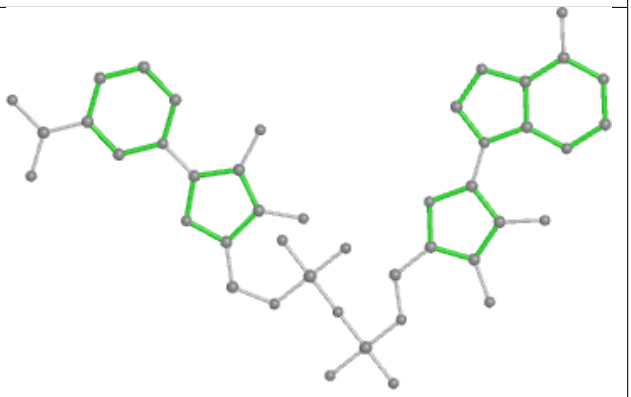
Bond lengths



Bond angles

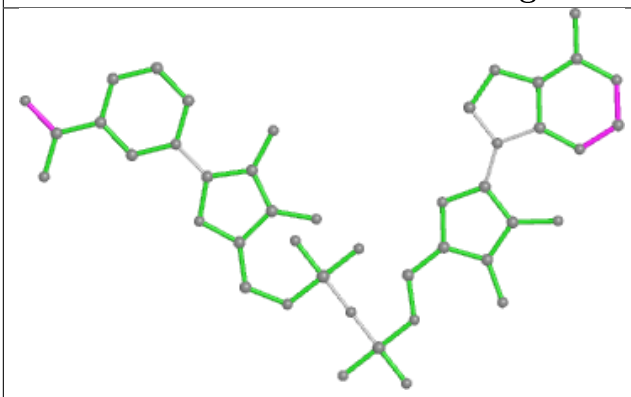


Torsions

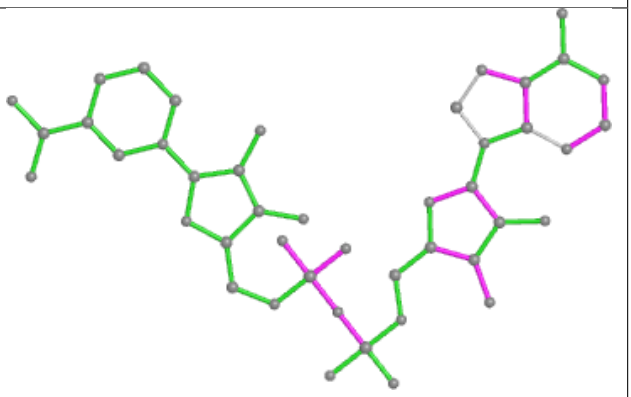


Rings

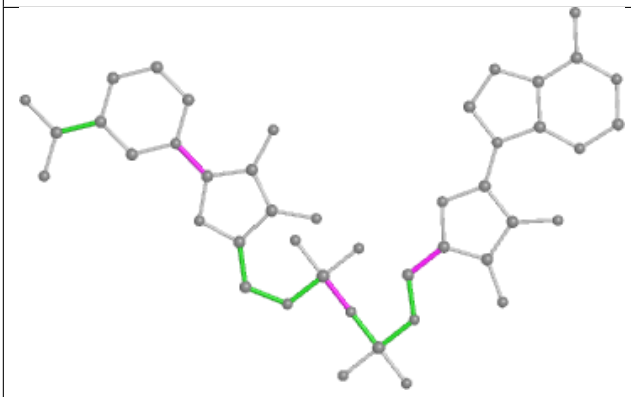
Ligand NAD D 400



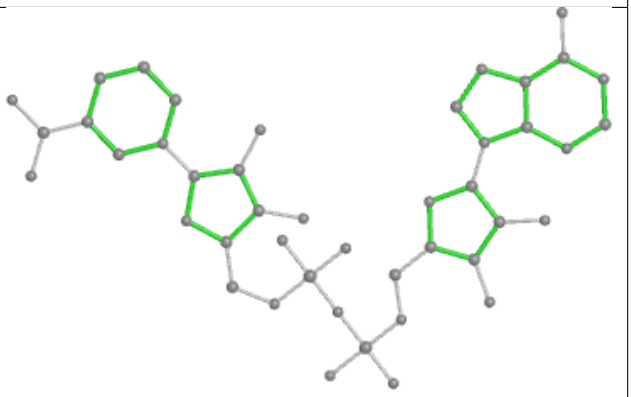
Bond lengths



Bond angles

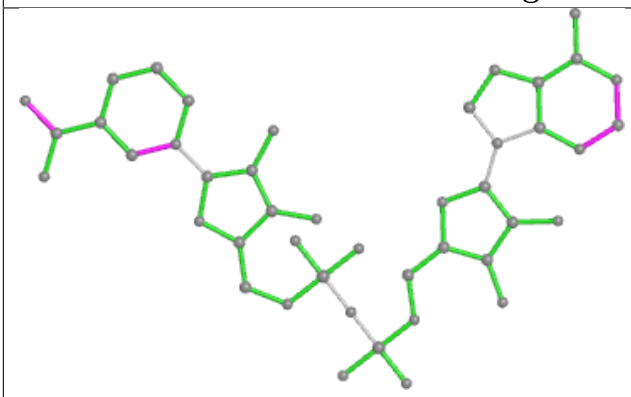


Torsions

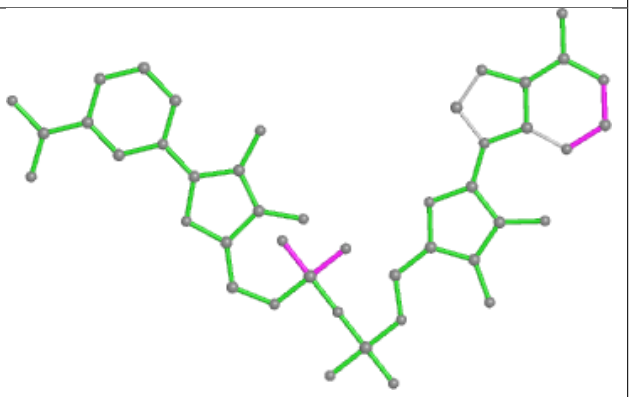


Rings

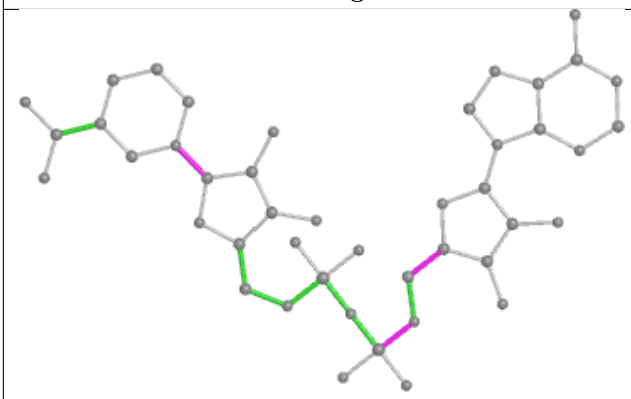
Ligand NAD F 400



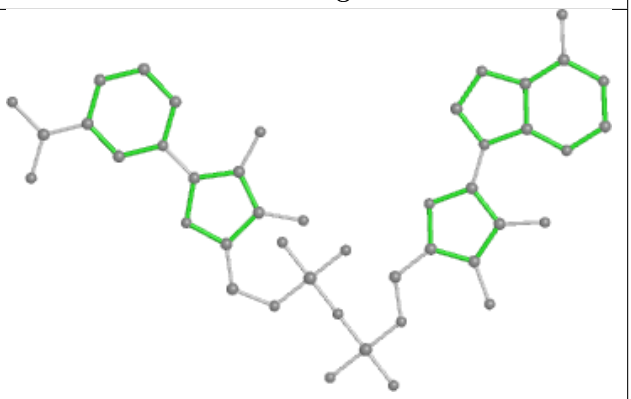
Bond lengths



Bond angles

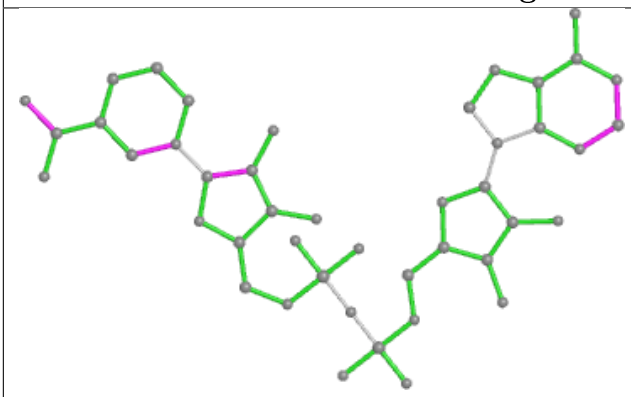


Torsions

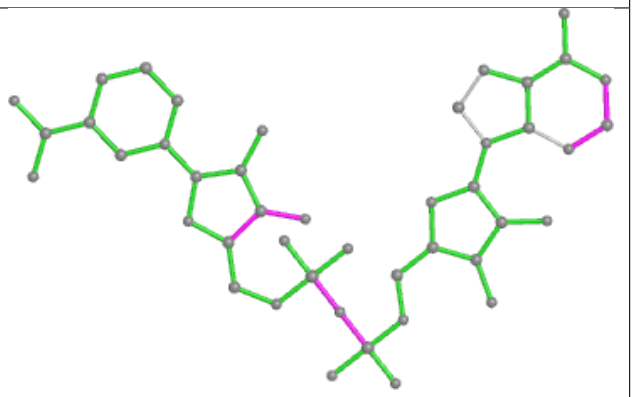


Rings

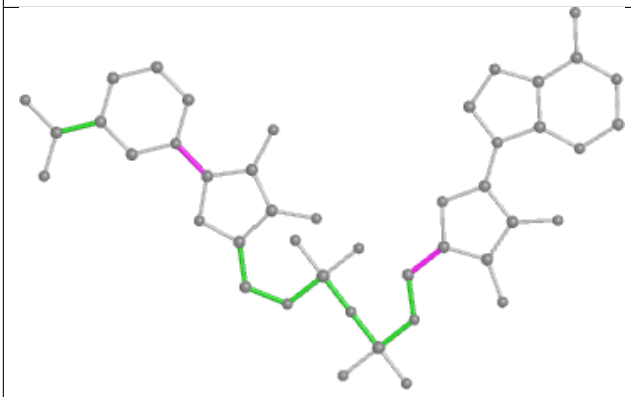
Ligand NAD G 400



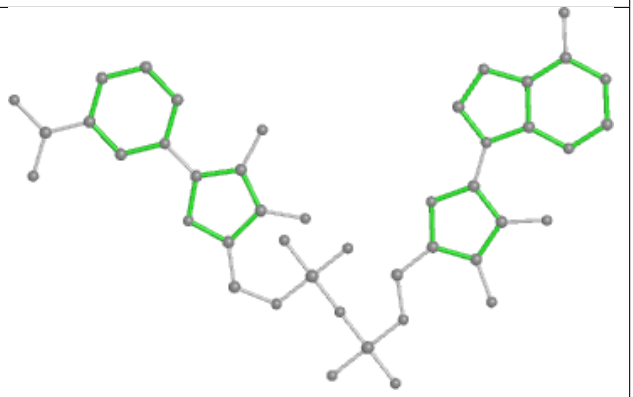
Bond lengths



Bond angles

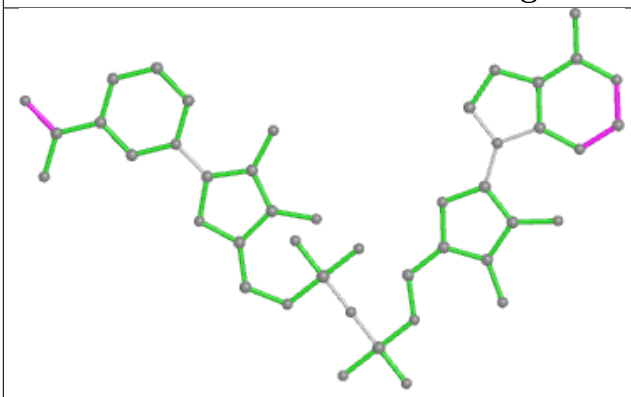


Torsions

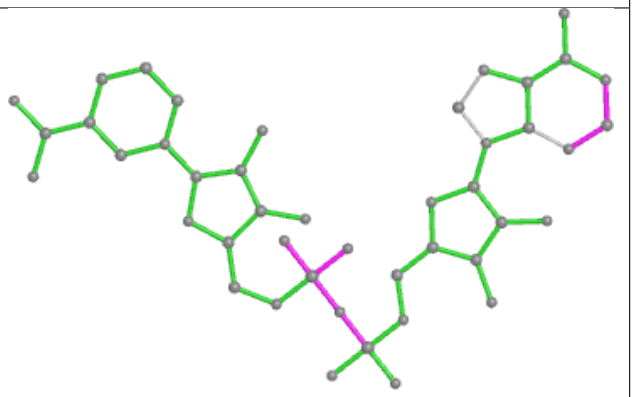


Rings

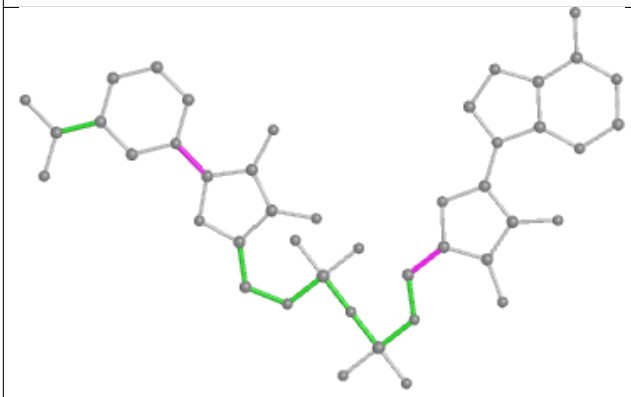
Ligand NAD C 400



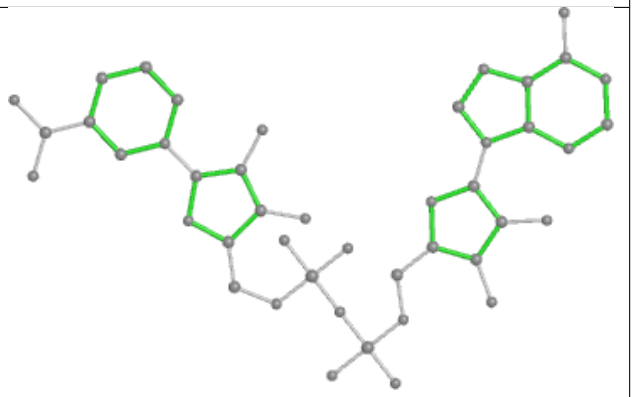
Bond lengths



Bond angles

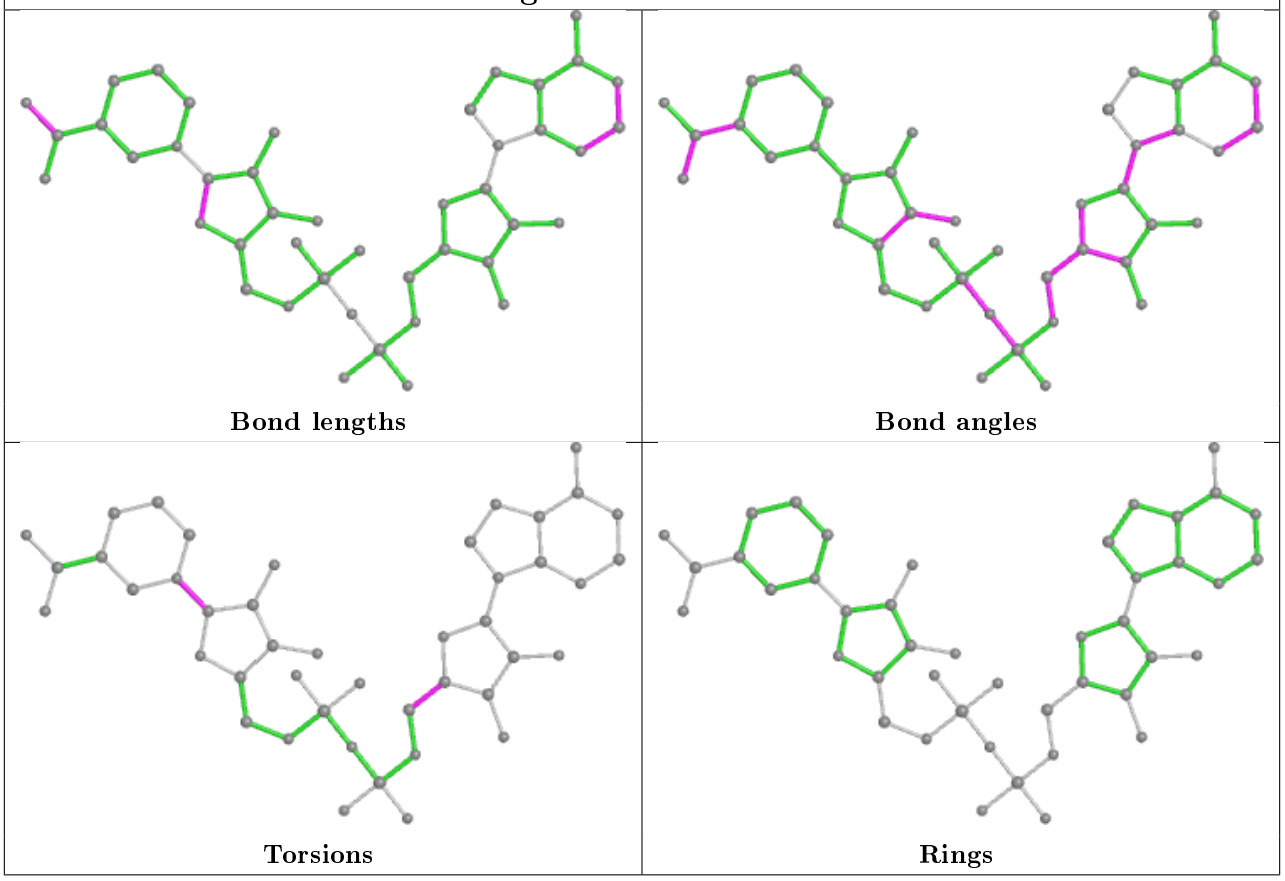


Torsions



Rings

Ligand NAD A 400



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	328/357 (91%)	-0.28	0 100 100	11, 19, 30, 37	0
1	B	328/357 (91%)	-0.15	6 (1%) 68 75	12, 21, 34, 40	0
1	C	328/357 (91%)	-0.04	7 (2%) 63 71	11, 23, 36, 43	0
1	D	328/357 (91%)	-0.22	1 (0%) 94 95	10, 21, 34, 42	0
1	E	328/357 (91%)	-0.25	0 100 100	12, 20, 31, 37	0
1	F	328/357 (91%)	-0.03	7 (2%) 63 71	11, 24, 37, 47	0
1	G	328/357 (91%)	0.01	10 (3%) 50 59	11, 23, 37, 47	0
1	H	328/357 (91%)	-0.22	2 (0%) 89 91	11, 20, 33, 43	0
All	All	2624/2856 (91%)	-0.15	33 (1%) 77 82	10, 21, 35, 47	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	ILE	4.5
1	C	65	LYS	4.0
1	F	44	ALA	3.7
1	C	62	ILE	3.6
1	C	50	ILE	3.4
1	G	118	LYS	3.4
1	D	50	ILE	3.4
1	C	33	VAL	3.3
1	F	101	VAL	3.1
1	G	33	VAL	3.1
1	B	9	GLY	3.0
1	F	110	ILE	2.9
1	F	52	ALA	2.9
1	F	92	TYR	2.7
1	B	61	LEU	2.7
1	G	48	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	49	ALA	2.6
1	G	47	LYS	2.6
1	G	101	VAL	2.5
1	B	50	ILE	2.5
1	G	92	TYR	2.5
1	H	50	ILE	2.5
1	B	3	LEU	2.4
1	G	38	ALA	2.3
1	B	36	ILE	2.3
1	C	84	VAL	2.3
1	F	48	TYR	2.2
1	B	30	VAL	2.2
1	H	51	GLU	2.1
1	G	66	ASP	2.1
1	C	48	TYR	2.1
1	C	3	LEU	2.1
1	G	57	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	ACY	A	402	4/4	0.89	0.13	53,53,53,53	0
5	EDO	E	403	4/4	0.89	0.14	50,52,53,53	0
5	EDO	G	402	4/4	0.91	0.14	39,41,41,44	0
6	K	D	403	1/1	0.92	0.14	73,73,73,73	0
3	EPE	G	401	15/15	0.94	0.10	40,42,50,51	0
3	EPE	H	401	15/15	0.94	0.13	37,39,45,48	0

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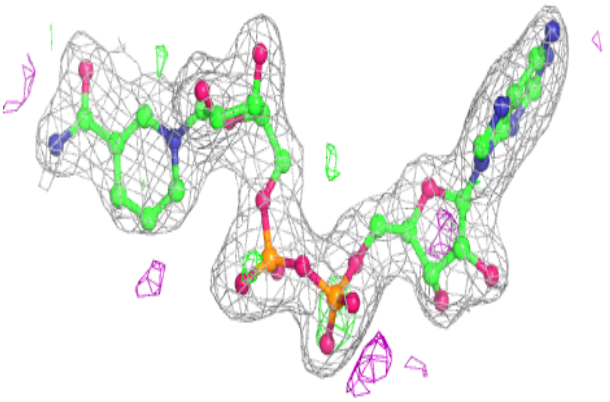
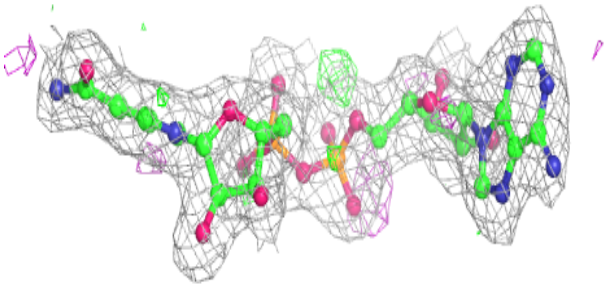
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	B	400	44/44	0.94	0.10	33,44,53,55	0
3	EPE	F	401	15/15	0.94	0.11	38,41,47,50	0
2	NAD	F	400	44/44	0.94	0.11	30,43,53,56	0
3	EPE	C	401	15/15	0.95	0.10	43,45,48,49	0
3	EPE	B	401	15/15	0.95	0.13	37,40,52,53	0
3	EPE	A	401	15/15	0.95	0.12	32,35,38,41	0
2	NAD	E	400	44/44	0.96	0.10	24,37,44,45	0
4	ACY	A	403	4/4	0.96	0.21	36,36,36,36	0
3	EPE	D	401	15/15	0.96	0.10	33,36,41,44	0
5	EDO	H	402	4/4	0.96	0.09	20,24,25,34	0
3	EPE	E	401	15/15	0.96	0.10	26,30,37,38	0
2	NAD	G	400	44/44	0.96	0.10	35,44,51,54	0
5	EDO	E	402	4/4	0.96	0.14	21,23,29,32	0
2	NAD	C	400	44/44	0.96	0.10	37,46,54,54	0
2	NAD	D	400	44/44	0.97	0.09	30,39,46,48	0
2	NAD	H	400	44/44	0.97	0.10	32,38,44,46	0
2	NAD	A	400	44/44	0.97	0.10	25,31,34,38	0
6	K	H	403	1/1	0.98	0.11	65,65,65,65	0
5	EDO	D	402	4/4	0.99	0.09	29,29,33,36	0

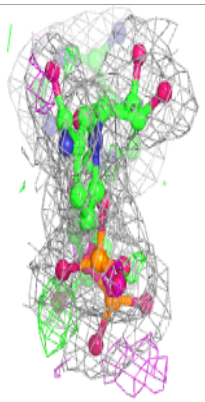
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 400:

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

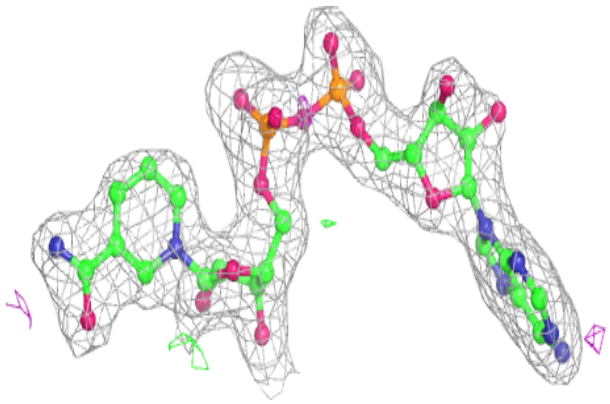


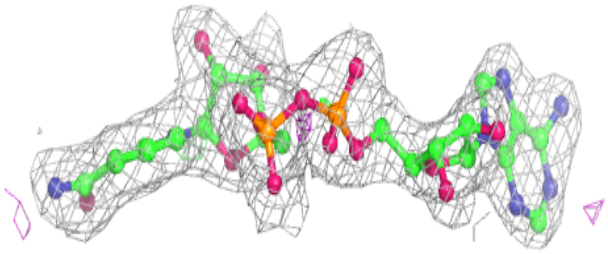


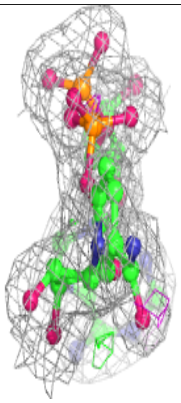


Electron density around NAD F 400:

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

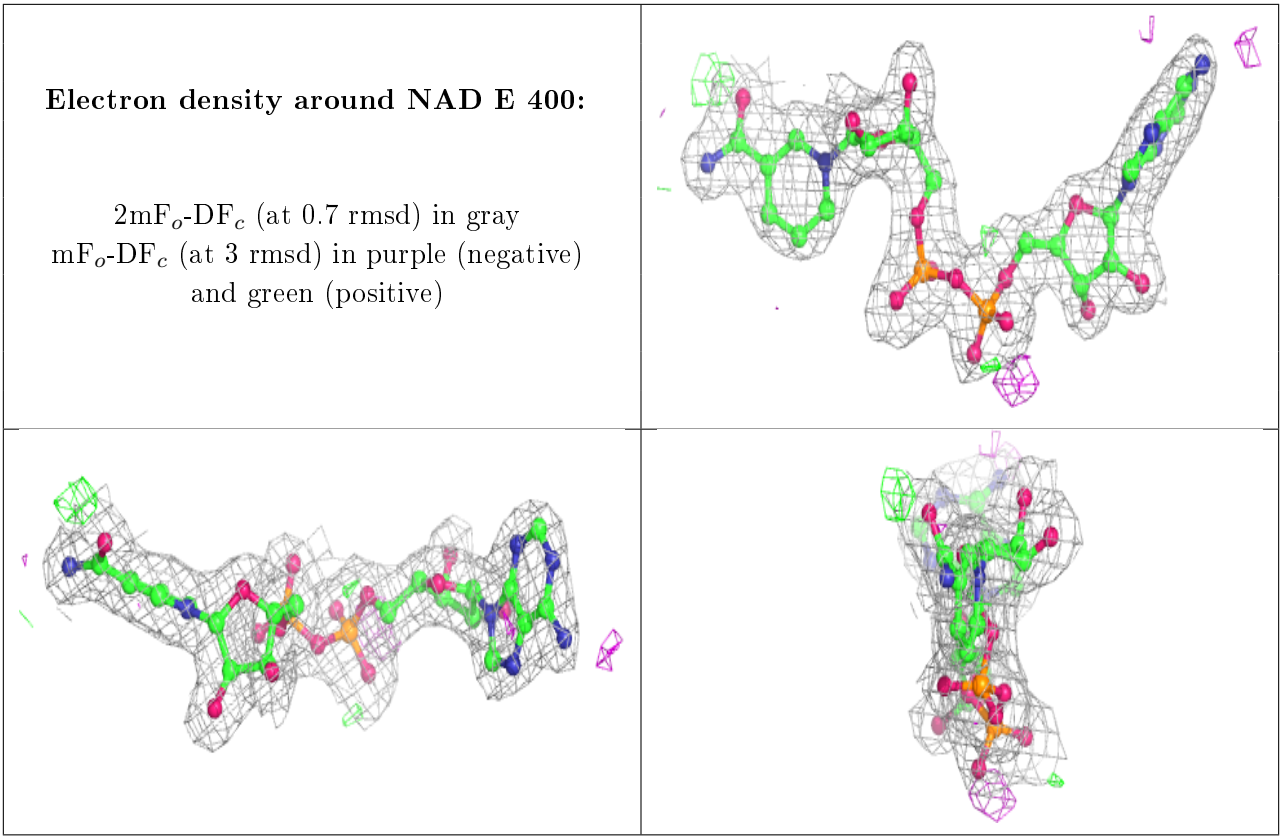






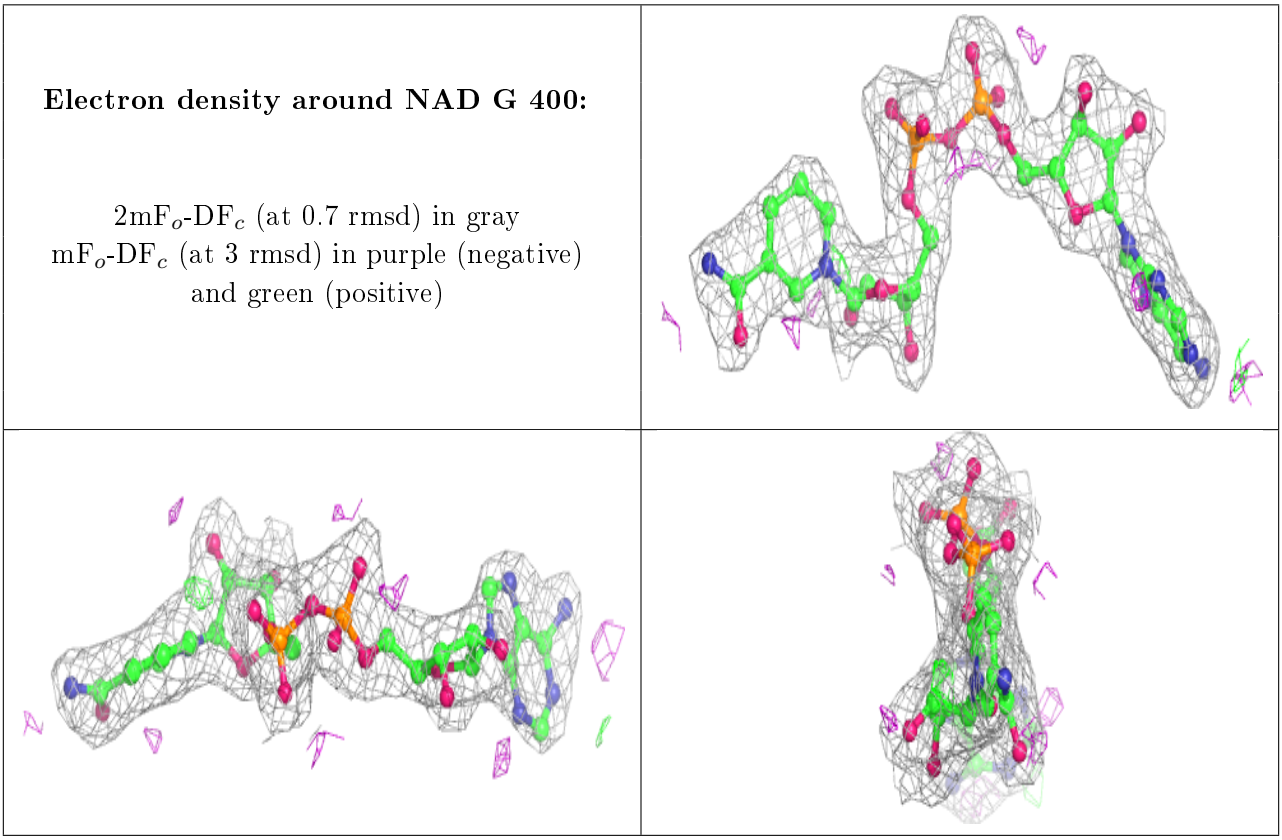
Electron density around NAD E 400:

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



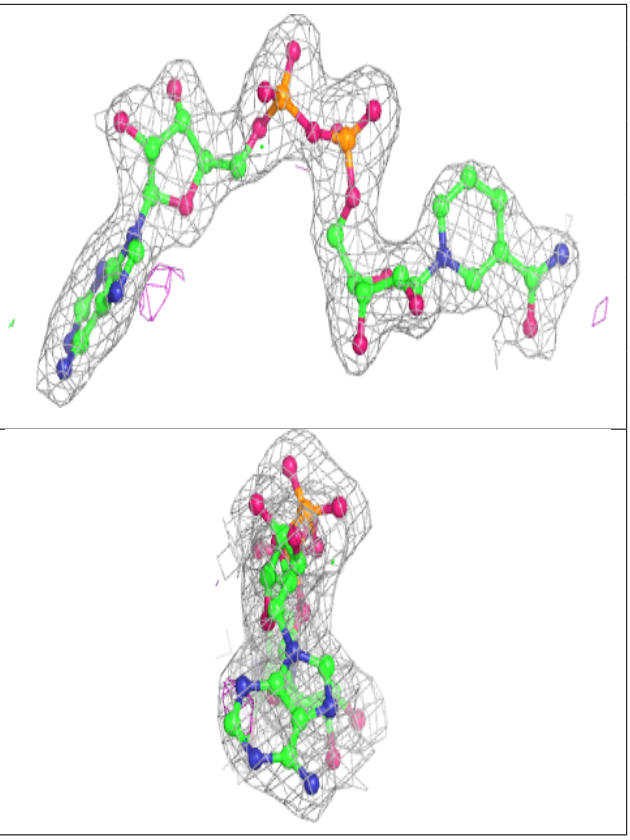
Electron density around NAD G 400:

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



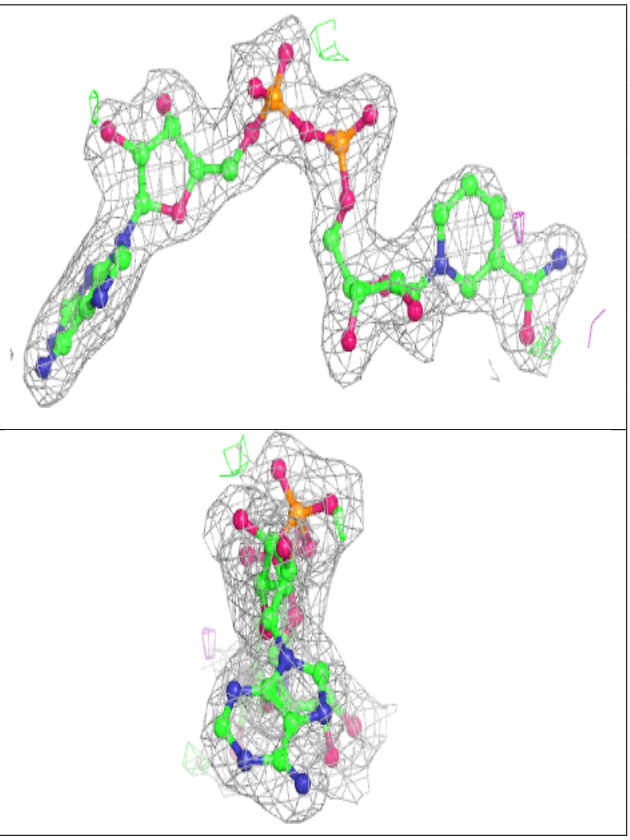
Electron density around NAD C 400:

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



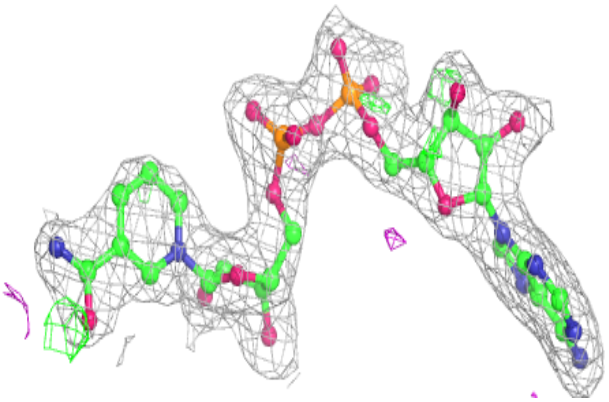
Electron density around NAD D 400:

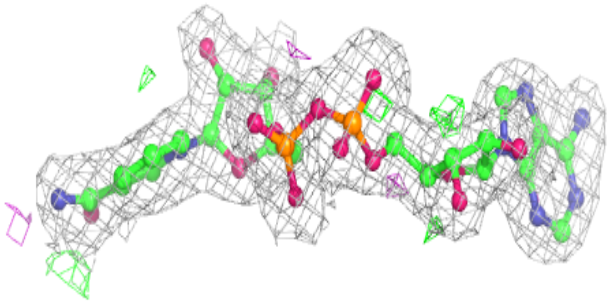
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

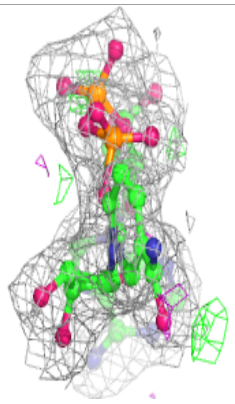


Electron density around NAD H 400:

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

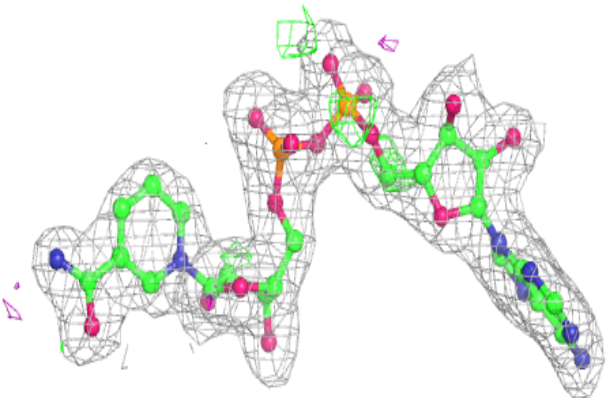


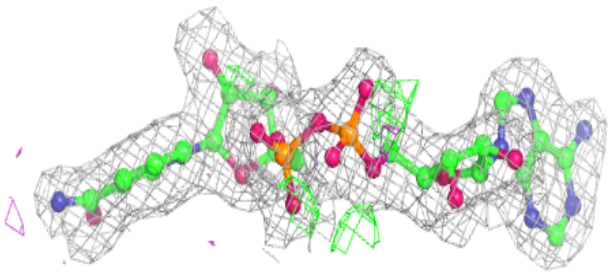


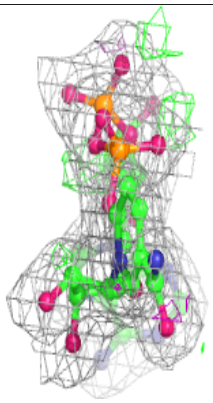


Electron density around NAD A 400:

$2mF_o$-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.