Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 02:24 AM EDT

PDB ID	:	2HAE
Title	:	Crystal structure of a putative malic enzyme (malate oxidoreductase)
Authors	:	Seetharaman, J.; Swaminathan, S.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-06-12
Resolution	:	3.13 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:

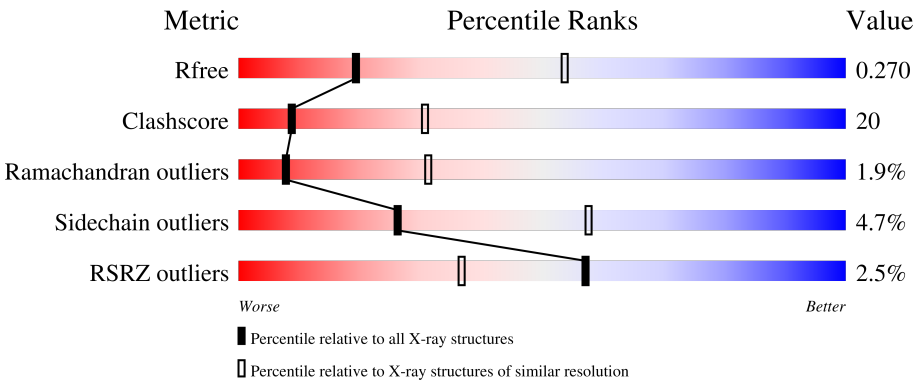
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	386	% 66% 28% • •
1	B	386	65% 30% • •
1	C	386	6% 60% 34% • •
1	D	386	3% 56% 37% • • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11756 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 Malate oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	373	2860	1826	483	540	11	0	0	0
1	B	373	2860	1826	483	540	11	0	0	0
1	C	373	2860	1826	483	540	11	0	0	0
1	D	373	2860	1826	483	540	11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q9WZ12
A	0	SER	-	cloning artifact	UNP Q9WZ12
A	1	LEU	-	cloning artifact	UNP Q9WZ12
A	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
A	377	GLU	-	cloning artifact	UNP Q9WZ12
A	378	GLY	-	cloning artifact	UNP Q9WZ12
A	379	HIS	-	cloning artifact	UNP Q9WZ12
A	380	HIS	-	cloning artifact	UNP Q9WZ12
A	381	HIS	-	cloning artifact	UNP Q9WZ12
A	382	HIS	-	cloning artifact	UNP Q9WZ12
A	383	HIS	-	cloning artifact	UNP Q9WZ12
A	384	HIS	-	cloning artifact	UNP Q9WZ12
B	-1	MET	-	cloning artifact	UNP Q9WZ12
B	0	SER	-	cloning artifact	UNP Q9WZ12
B	1	LEU	-	cloning artifact	UNP Q9WZ12
B	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
B	377	GLU	-	cloning artifact	UNP Q9WZ12
B	378	GLY	-	cloning artifact	UNP Q9WZ12
B	379	HIS	-	cloning artifact	UNP Q9WZ12
B	380	HIS	-	cloning artifact	UNP Q9WZ12
B	381	HIS	-	cloning artifact	UNP Q9WZ12

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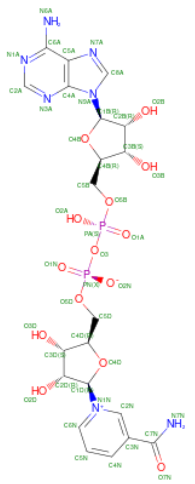
Chain	Residue	Modelled	Actual	Comment	Reference
B	382	HIS	-	cloning artifact	UNP Q9WZ12
B	383	HIS	-	cloning artifact	UNP Q9WZ12
B	384	HIS	-	cloning artifact	UNP Q9WZ12
C	-1	MET	-	cloning artifact	UNP Q9WZ12
C	0	SER	-	cloning artifact	UNP Q9WZ12
C	1	LEU	-	cloning artifact	UNP Q9WZ12
C	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
C	377	GLU	-	cloning artifact	UNP Q9WZ12
C	378	GLY	-	cloning artifact	UNP Q9WZ12
C	379	HIS	-	cloning artifact	UNP Q9WZ12
C	380	HIS	-	cloning artifact	UNP Q9WZ12
C	381	HIS	-	cloning artifact	UNP Q9WZ12
C	382	HIS	-	cloning artifact	UNP Q9WZ12
C	383	HIS	-	cloning artifact	UNP Q9WZ12
C	384	HIS	-	cloning artifact	UNP Q9WZ12
D	-1	MET	-	cloning artifact	UNP Q9WZ12
D	0	SER	-	cloning artifact	UNP Q9WZ12
D	1	LEU	-	cloning artifact	UNP Q9WZ12
D	6	LEU	ILE	SEE REMARK 999	UNP Q9WZ12
D	377	GLU	-	cloning artifact	UNP Q9WZ12
D	378	GLY	-	cloning artifact	UNP Q9WZ12
D	379	HIS	-	cloning artifact	UNP Q9WZ12
D	380	HIS	-	cloning artifact	UNP Q9WZ12
D	381	HIS	-	cloning artifact	UNP Q9WZ12
D	382	HIS	-	cloning artifact	UNP Q9WZ12
D	383	HIS	-	cloning artifact	UNP Q9WZ12
D	384	HIS	-	cloning artifact	UNP Q9WZ12

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

NAD



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		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

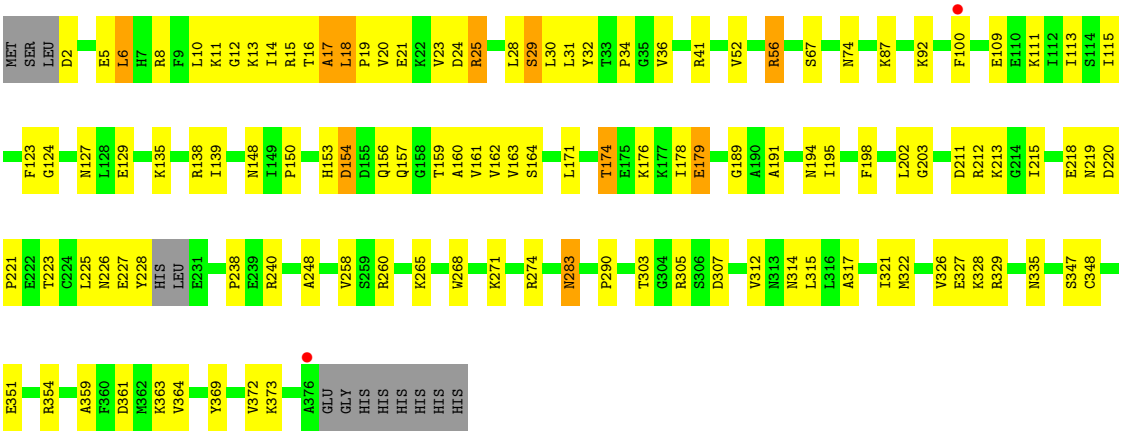
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	41	Total	O	0	0
			41	41		
4	C	46	Total	O	0	0
			46	46		
4	D	52	Total	O	0	0
			52	52		

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.

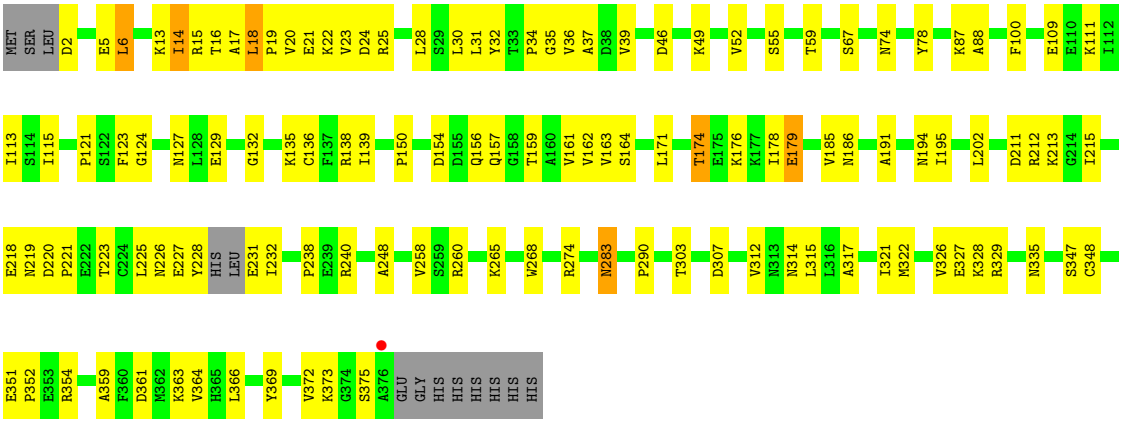
• Molecule 1: Malate oxidoreductase

Chain A:



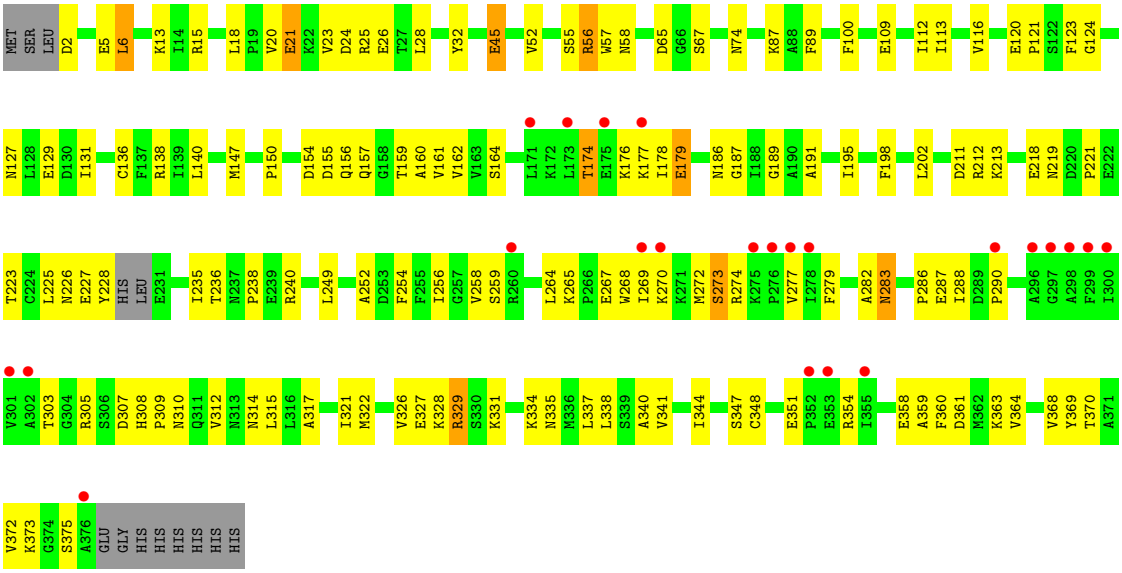
• Molecule 1: Malate oxidoreductase

Chain B:



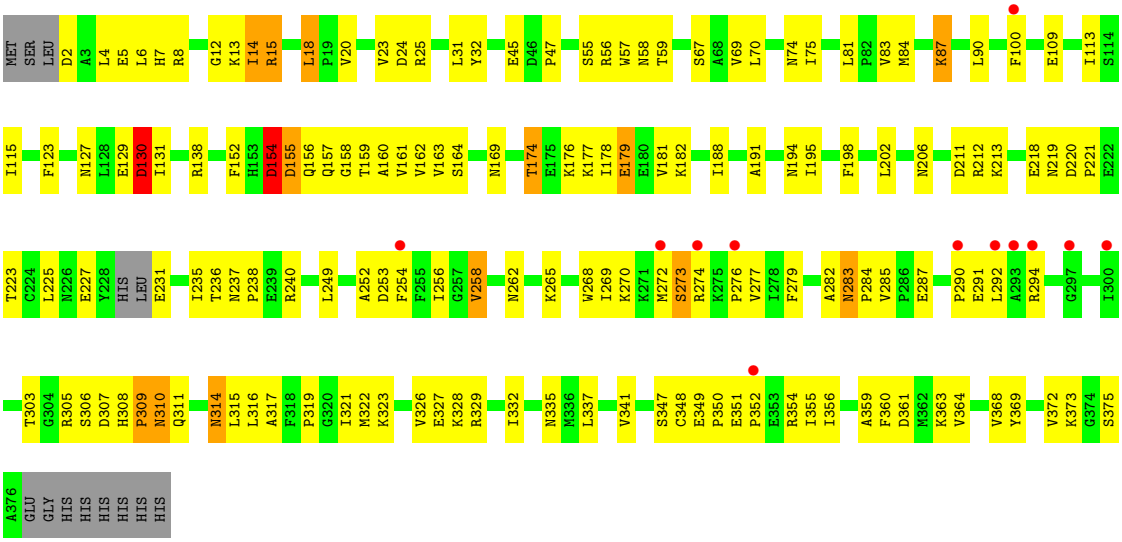
• Molecule 1: Malate oxidoreductase

Chain C:



- Molecule 1: Malate oxidoreductase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	145.80Å 145.80Å 159.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.13 49.47 – 3.13	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.13) 94.9 (49.47-3.13)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.282 0.234 , 0.270	Depositor DCC
R_{free} test set	2425 reflections (7.22%)	wwPDB-VP
Wilson B-factor (Å^2)	72.4	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11756	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/2910	0.65	0/3942
1	B	0.47	0/2910	0.65	0/3942
1	C	0.48	0/2910	0.66	0/3942
1	D	0.49	0/2910	0.66	3/3942 (0.1%)
All	All	0.48	0/11640	0.65	3/15768 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	155	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	130	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	154	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	316	LEU	Peptide

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	2860	0	2920	116	0
1	B	2860	0	2920	125	0
1	C	2860	0	2920	127	0
1	D	2860	0	2920	158	0
2	A	44	0	26	10	0
2	B	44	0	26	13	0
2	C	44	0	26	12	0
3	D	1	0	0	0	0
4	A	44	0	0	12	0
4	B	41	0	0	16	0
4	C	46	0	0	18	0
4	D	52	0	0	23	0
All	All	11756	0	11758	478	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 20.

All (478) 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)
2:A:501:NAD:H6N	1:B:283:ASN:HD22	1.13	1.11
1:B:32:TYR:OH	1:D:87:LYS:HE3	1.58	1.01
1:D:15:ARG:HG2	1:D:15:ARG:HH11	1.28	0.94
1:A:159:THR:CG2	2:B:501:NAD:H72N	1.79	0.94
2:A:501:NAD:C6N	1:B:283:ASN:HD22	1.82	0.92
1:B:185:VAL:HG12	4:B:523:HOH:O	1.70	0.92
1:A:30:LEU:HD13	1:C:6:LEU:HG	1.51	0.91
2:A:501:NAD:H6N	1:B:283:ASN:ND2	1.87	0.89
1:C:249:LEU:HD22	1:C:272:MET:SD	2.14	0.88
1:A:13:LYS:HE2	4:C:532:HOH:O	1.75	0.86
1:A:283:ASN:HD22	2:B:501:NAD:H6N	1.38	0.85
1:C:177:LYS:HG3	4:C:521:HOH:O	1.74	0.85
1:C:358:GLU:HB2	4:C:519:HOH:O	1.76	0.85
1:D:69:VAL:HA	1:D:130:ASP:OD2	1.76	0.85
1:B:328:LYS:HE3	1:B:375:SER:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASP:O	1:C:6:LEU:HD23	1.75	0.84
1:D:67:SER:HA	1:D:74:ASN:OD1	1.78	0.83
1:A:159:THR:HG23	2:B:501:NAD:H72N	1.43	0.83
1:C:283:ASN:HB3	2:C:501:NAD:H6N	1.60	0.82
1:C:360:PHE:HB2	4:C:519:HOH:O	1.79	0.81
1:D:350:PRO:HG3	4:D:834:HOH:O	1.81	0.81
1:B:231:GLU:HB3	4:B:510:HOH:O	1.81	0.80
1:C:267:GLU:HA	4:C:540:HOH:O	1.82	0.80
1:B:32:TYR:OH	1:D:87:LYS:CE	2.29	0.80
1:A:67:SER:HA	1:A:74:ASN:OD1	1.83	0.79
1:D:15:ARG:HG2	1:D:15:ARG:NH1	1.90	0.79
1:A:321:ILE:HA	1:A:372:VAL:HG21	1.65	0.77
1:A:32:TYR:OH	1:C:87:LYS:HE2	1.84	0.77
1:D:291:GLU:HB2	4:D:804:HOH:O	1.84	0.77
1:C:140:LEU:HB2	4:C:533:HOH:O	1.84	0.77
1:D:292:LEU:HA	4:D:851:HOH:O	1.83	0.77
1:D:284:PRO:HA	4:D:821:HOH:O	1.84	0.77
1:B:232:ILE:HG12	4:B:510:HOH:O	1.85	0.77
1:B:67:SER:HA	1:B:74:ASN:OD1	1.85	0.76
1:A:363:LYS:HE3	1:B:363:LYS:HE3	1.69	0.75
1:B:55:SER:O	1:B:59:THR:HG23	1.87	0.75
1:C:328:LYS:HE3	1:C:375:SER:O	1.86	0.75
1:B:23:VAL:HG12	1:D:360:PHE:HE1	1.50	0.75
1:B:20:VAL:HG12	1:B:21:GLU:N	2.02	0.74
1:B:87:LYS:HE2	1:D:32:TYR:OH	1.87	0.73
1:A:203:GLY:HA3	4:A:524:HOH:O	1.87	0.73
1:C:67:SER:HA	1:C:74:ASN:OD1	1.88	0.72
1:D:328:LYS:HE3	1:D:375:SER:O	1.90	0.72
1:A:18:LEU:HD12	1:A:18:LEU:H	1.55	0.72
1:A:87:LYS:HE2	1:C:32:TYR:OH	1.89	0.72
2:A:501:NAD:H72N	1:B:159:THR:CG2	2.02	0.72
1:B:321:ILE:HA	1:B:372:VAL:HG21	1.70	0.71
1:D:2:ASP:HB3	1:D:5:GLU:OE1	1.89	0.71
1:C:351:GLU:HG3	1:C:354:ARG:HB3	1.72	0.71
1:C:269:ILE:HG21	4:C:511:HOH:O	1.89	0.71
1:D:18:LEU:HD13	1:D:20:VAL:O	1.91	0.71
1:D:290:PRO:HA	4:D:835:HOH:O	1.90	0.71
2:A:501:NAD:H61A	1:B:260:ARG:HH21	1.37	0.71
1:A:21:GLU:HB2	1:B:15:ARG:NH1	2.05	0.70
1:D:211:ASP:HB3	4:D:816:HOH:O	1.90	0.70
1:D:174:THR:HG23	1:D:176:LYS:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:O	1:A:221:PRO:HD3	1.92	0.69
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.57	0.69
1:D:87:LYS:NZ	1:D:129:GLU:OE2	2.24	0.69
1:A:159:THR:CG2	2:B:501:NAD:N7N	2.54	0.69
1:B:219:ASN:O	1:B:221:PRO:HD3	1.93	0.69
1:C:282:ALA:HA	2:C:501:NAD:H1D	1.75	0.69
1:C:159:THR:CG2	2:C:501:NAD:H72N	2.04	0.69
1:C:321:ILE:HA	1:C:372:VAL:HG21	1.74	0.69
1:B:30:LEU:HD13	1:D:6:LEU:HD12	1.75	0.69
1:D:321:ILE:HA	1:D:372:VAL:HG21	1.74	0.68
1:D:237:ASN:HB3	4:D:829:HOH:O	1.93	0.68
1:A:283:ASN:HD22	2:B:501:NAD:C6N	2.06	0.68
1:C:23:VAL:HG11	1:C:28:LEU:HD21	1.75	0.68
1:C:174:THR:HG23	1:C:176:LYS:HG3	1.76	0.68
1:D:23:VAL:HG12	1:D:24:ASP:N	2.08	0.68
1:A:19:PRO:HG2	1:A:20:VAL:H	1.57	0.68
1:B:18:LEU:HD12	1:B:18:LEU:H	1.58	0.68
1:D:156:GLN:HB3	1:D:194:ASN:ND2	2.07	0.67
1:B:351:GLU:HG3	1:B:354:ARG:HB3	1.77	0.67
1:D:70:LEU:N	1:D:130:ASP:OD2	2.27	0.66
1:A:174:THR:HG23	1:A:176:LYS:HG3	1.78	0.66
1:C:57:TRP:CE3	1:C:58:ASN:HB2	2.31	0.65
1:D:219:ASN:O	1:D:221:PRO:HD3	1.95	0.65
1:B:174:THR:HG23	1:B:176:LYS:HG3	1.79	0.65
1:D:2:ASP:HB3	1:D:5:GLU:CD	2.16	0.65
1:D:109:GLU:OE2	1:D:138:ARG:HD2	1.96	0.65
1:B:20:VAL:HG12	1:B:21:GLU:H	1.61	0.65
1:B:32:TYR:C	1:B:36:VAL:HG12	2.18	0.65
1:A:290:PRO:HG3	1:A:303:THR:HG21	1.77	0.65
1:C:191:ALA:O	1:C:195:ILE:HG13	1.97	0.65
1:C:24:ASP:OD2	1:C:26:GLU:HB3	1.98	0.64
1:A:328:LYS:O	1:A:328:LYS:HG2	1.97	0.64
1:C:322:MET:O	1:C:326:VAL:HG23	1.98	0.64
1:B:290:PRO:HG3	1:B:303:THR:HG21	1.80	0.63
1:C:159:THR:HG23	2:C:501:NAD:H72N	1.63	0.63
1:C:249:LEU:O	1:C:272:MET:HG2	1.99	0.63
1:A:219:ASN:CB	4:A:540:HOH:O	2.46	0.62
1:D:69:VAL:HG11	1:D:75:ILE:HD11	1.80	0.62
1:C:351:GLU:CG	1:C:354:ARG:HB3	2.28	0.62
1:D:258:VAL:HG13	1:D:258:VAL:O	1.99	0.62
2:A:501:NAD:H72N	1:B:159:THR:HG23	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:ND2	2:B:501:NAD:H6N	2.13	0.62
1:A:351:GLU:HG3	1:A:354:ARG:HB3	1.80	0.62
1:B:13:LYS:HE2	4:D:825:HOH:O	1.98	0.62
1:B:32:TYR:CZ	1:D:87:LYS:HE3	2.35	0.62
1:D:314:ASN:O	1:D:317:ALA:N	2.32	0.62
1:A:271:LYS:HB2	4:A:512:HOH:O	1.99	0.61
1:C:189:GLY:HA3	2:C:501:NAD:O5B	1.99	0.61
1:D:351:GLU:HG3	1:D:354:ARG:HB3	1.83	0.61
1:C:219:ASN:O	1:C:221:PRO:HD3	1.99	0.61
1:C:6:LEU:HD23	1:C:6:LEU:H	1.65	0.61
4:B:511:HOH:O	1:D:14:ILE:HG12	2.01	0.61
1:A:258:VAL:O	1:A:258:VAL:HG13	2.01	0.61
1:D:283:ASN:HB2	4:D:821:HOH:O	2.01	0.60
1:B:156:GLN:HB3	1:B:194:ASN:ND2	2.15	0.60
1:B:157:GLN:O	1:B:161:VAL:HG23	2.01	0.60
1:B:258:VAL:O	1:B:258:VAL:HG13	2.02	0.60
1:C:287:GLU:HG2	4:C:535:HOH:O	2.01	0.60
1:B:109:GLU:O	1:B:113:ILE:HG13	2.01	0.59
1:A:157:GLN:O	1:A:161:VAL:HG23	2.03	0.59
1:A:159:THR:HG23	2:B:501:NAD:N7N	2.17	0.59
1:A:219:ASN:HB2	4:A:540:HOH:O	2.02	0.59
1:B:123:PHE:CE1	1:D:100:PHE:HE2	2.20	0.59
1:B:23:VAL:HG12	1:D:360:PHE:CE1	2.34	0.59
1:C:272:MET:O	1:C:273:SER:O	2.21	0.59
1:C:235:ILE:HG13	1:C:236:THR:HG23	1.84	0.59
1:C:6:LEU:N	1:C:6:LEU:CD2	2.66	0.59
1:C:65:ASP:HB2	4:C:514:HOH:O	2.02	0.58
1:D:270:LYS:HG3	4:D:802:HOH:O	2.03	0.58
1:B:13:LYS:HG2	1:D:31:LEU:HD22	1.83	0.58
1:D:90:LEU:HD13	1:D:315:LEU:HD13	1.86	0.58
1:A:56:ARG:HG2	1:A:56:ARG:HH11	1.69	0.58
1:B:15:ARG:HH11	1:B:15:ARG:HG2	1.68	0.58
1:D:231:GLU:N	4:D:803:HOH:O	2.36	0.58
1:A:138:ARG:HD3	4:A:522:HOH:O	2.01	0.58
1:D:2:ASP:OD2	1:D:5:GLU:HG3	2.03	0.58
1:D:177:LYS:O	1:D:181:VAL:HG13	2.03	0.58
1:A:156:GLN:HB3	1:A:194:ASN:ND2	2.19	0.58
1:B:366:LEU:HD12	4:B:535:HOH:O	2.03	0.58
1:B:46:ASP:HB3	1:B:49:LYS:HG2	1.85	0.58
1:A:2:ASP:N	4:A:504:HOH:O	2.37	0.58
1:D:253:ASP:HA	4:D:811:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:HG2	1:C:15:ARG:NH1	2.19	0.58
1:D:182:LYS:HG3	1:D:206:ASN:ND2	2.19	0.57
1:B:55:SER:OG	1:D:12:GLY:HA3	2.05	0.57
4:B:511:HOH:O	1:D:14:ILE:HA	2.03	0.57
1:D:294:ARG:CB	4:D:809:HOH:O	2.52	0.57
1:D:314:ASN:O	1:D:317:ALA:HB3	2.03	0.57
1:C:45:GLU:HB3	4:C:536:HOH:O	2.03	0.57
1:D:249:LEU:HD22	1:D:272:MET:SD	2.44	0.57
1:D:290:PRO:HG3	1:D:303:THR:HG21	1.85	0.57
1:A:6:LEU:N	1:A:6:LEU:CD2	2.67	0.56
1:C:155:ASP:HB3	4:C:503:HOH:O	2.05	0.56
1:C:258:VAL:HG13	1:C:258:VAL:O	2.04	0.56
1:C:273:SER:HB2	4:C:534:HOH:O	2.05	0.56
1:D:157:GLN:O	1:D:161:VAL:HG23	2.05	0.56
1:A:8:ARG:HH11	1:C:52:VAL:HG13	1.71	0.56
1:C:290:PRO:HG3	1:C:303:THR:HG21	1.88	0.56
1:A:10:LEU:O	1:A:11:LYS:HB2	2.05	0.56
1:B:30:LEU:HD13	1:D:6:LEU:CD1	2.36	0.56
1:A:87:LYS:NZ	4:A:536:HOH:O	2.39	0.56
1:C:307:ASP:HB3	1:C:308:HIS:CD2	2.40	0.56
1:D:18:LEU:HD12	1:D:18:LEU:H	1.70	0.56
1:B:20:VAL:CG1	1:B:21:GLU:N	2.69	0.56
1:B:31:LEU:HD22	1:D:13:LYS:HD3	1.88	0.56
1:C:354:ARG:NH2	4:C:543:HOH:O	2.39	0.56
1:C:348:CYS:HB2	1:C:354:ARG:HH21	1.71	0.56
1:D:57:TRP:CE3	1:D:58:ASN:HB2	2.41	0.56
1:A:87:LYS:HE3	1:A:129:GLU:CD	2.27	0.55
1:C:327:GLU:C	1:C:329:ARG:H	2.10	0.55
1:D:169:ASN:HA	4:D:834:HOH:O	2.06	0.55
1:D:314:ASN:OD1	1:D:314:ASN:N	2.32	0.55
1:C:87:LYS:HE3	1:C:129:GLU:CD	2.27	0.55
1:A:18:LEU:HD12	1:A:18:LEU:N	2.21	0.55
1:D:23:VAL:CG1	1:D:24:ASP:N	2.69	0.55
1:D:138:ARG:HD3	4:D:820:HOH:O	2.07	0.55
1:C:186:ASN:HB3	4:C:535:HOH:O	2.06	0.54
1:D:282:ALA:HB2	1:D:287:GLU:OE2	2.06	0.54
1:B:34:PRO:HG3	1:D:305:ARG:HH22	1.72	0.54
1:C:315:LEU:HD23	1:C:359:ALA:CB	2.36	0.54
1:C:57:TRP:CZ3	1:C:58:ASN:HB2	2.42	0.54
1:D:361:ASP:OD1	1:D:363:LYS:HB2	2.08	0.54
1:C:23:VAL:CG1	1:C:28:LEU:HD21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LYS:HE3	1:C:129:GLU:OE1	2.07	0.54
1:D:15:ARG:HH11	1:D:15:ARG:CG	2.10	0.54
1:D:138:ARG:NH1	1:D:138:ARG:HB2	2.23	0.54
1:C:112:ILE:O	1:C:116:VAL:HG23	2.07	0.54
1:D:23:VAL:HG12	1:D:24:ASP:H	1.72	0.54
1:A:6:LEU:N	1:A:6:LEU:HD23	2.21	0.54
1:A:21:GLU:HB2	1:B:15:ARG:HH11	1.73	0.54
1:B:20:VAL:CG1	1:B:21:GLU:H	2.21	0.53
1:D:138:ARG:HB2	1:D:138:ARG:CZ	2.39	0.53
1:D:174:THR:HG23	1:D:176:LYS:H	1.73	0.53
1:B:231:GLU:N	4:B:517:HOH:O	2.41	0.53
1:D:191:ALA:O	1:D:195:ILE:HG13	2.09	0.53
1:B:100:PHE:CZ	1:D:100:PHE:HB2	2.44	0.53
1:C:315:LEU:HD23	1:C:359:ALA:HB1	1.91	0.52
1:B:328:LYS:NZ	4:B:515:HOH:O	2.40	0.52
1:A:2:ASP:OD2	1:A:5:GLU:HG3	2.09	0.52
1:C:2:ASP:HB3	1:C:5:GLU:OE1	2.10	0.52
1:C:109:GLU:O	1:C:113:ILE:HG13	2.08	0.52
1:A:271:LYS:HE3	4:A:512:HOH:O	2.09	0.52
1:C:6:LEU:HD23	1:C:6:LEU:N	2.24	0.52
1:A:14:ILE:O	1:A:15:ARG:HG3	2.10	0.52
1:B:13:LYS:HD3	1:D:31:LEU:HD22	1.92	0.52
1:A:159:THR:CB	2:B:501:NAD:H72N	2.22	0.52
1:A:6:LEU:HD23	1:A:6:LEU:H	1.75	0.52
1:B:363:LYS:HA	4:B:535:HOH:O	2.09	0.52
1:D:328:LYS:NZ	4:D:831:HOH:O	2.42	0.52
1:A:109:GLU:O	1:A:113:ILE:HG13	2.10	0.51
1:A:159:THR:O	1:A:163:VAL:HG23	2.10	0.51
1:B:100:PHE:HB2	1:D:100:PHE:CZ	2.46	0.51
1:D:178:ILE:HG23	1:D:179:GLU:N	2.26	0.51
1:A:159:THR:OG1	2:B:501:NAD:N7N	2.43	0.51
1:A:219:ASN:HB3	4:A:540:HOH:O	2.06	0.51
1:B:228:TYR:HA	4:B:510:HOH:O	2.10	0.51
1:B:327:GLU:C	1:B:329:ARG:H	2.13	0.51
1:D:327:GLU:C	1:D:329:ARG:H	2.12	0.51
1:D:235:ILE:HG13	1:D:236:THR:HG23	1.92	0.51
1:D:109:GLU:O	1:D:113:ILE:HG13	2.11	0.51
1:A:138:ARG:HB2	1:A:138:ARG:CZ	2.41	0.51
1:A:322:MET:O	1:A:326:VAL:HG23	2.10	0.51
1:D:23:VAL:CG1	1:D:24:ASP:H	2.23	0.51
1:A:164:SER:HB3	1:A:202:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:VAL:HG13	1:D:8:ARG:HH11	1.76	0.50
1:A:87:LYS:HE2	1:C:32:TYR:HH	1.76	0.50
2:A:501:NAD:H6N	1:B:283:ASN:HB3	1.93	0.50
1:C:109:GLU:OE2	1:C:138:ARG:HD2	2.12	0.50
1:D:162:VAL:HG22	1:D:317:ALA:HB2	1.93	0.50
1:D:272:MET:O	1:D:273:SER:O	2.29	0.50
1:A:260:ARG:HH21	2:B:501:NAD:H61A	1.58	0.50
1:B:6:LEU:N	1:B:6:LEU:HD23	2.27	0.50
1:B:19:PRO:HG2	1:B:20:VAL:H	1.75	0.50
1:B:164:SER:HB3	1:B:202:LEU:HD11	1.94	0.50
1:D:294:ARG:HB3	4:D:809:HOH:O	2.10	0.50
1:D:351:GLU:CG	1:D:354:ARG:HB3	2.41	0.50
1:B:87:LYS:HE3	1:B:129:GLU:CD	2.32	0.50
1:D:156:GLN:HB3	1:D:194:ASN:HD21	1.77	0.50
1:C:211:ASP:CG	1:C:212:ARG:H	2.15	0.50
1:D:174:THR:CG2	1:D:176:LYS:H	2.25	0.50
1:A:14:ILE:C	1:A:15:ARG:HG3	2.33	0.50
1:B:14:ILE:C	1:B:15:ARG:HG3	2.31	0.50
1:A:171:LEU:O	1:A:174:THR:HG22	2.11	0.50
1:D:55:SER:O	1:D:56:ARG:C	2.50	0.50
1:A:138:ARG:HB2	1:A:138:ARG:NH1	2.27	0.49
1:A:111:LYS:O	1:A:115:ILE:HG13	2.13	0.49
1:D:211:ASP:CG	1:D:212:ARG:H	2.15	0.49
1:C:187:GLY:HA2	2:C:501:NAD:N3A	2.28	0.49
1:B:159:THR:O	1:B:163:VAL:HG23	2.12	0.49
1:B:238:PRO:C	1:B:240:ARG:H	2.16	0.49
1:B:78:TYR:CG	1:D:47:PRO:HB3	2.47	0.49
1:B:213:LYS:O	1:B:223:THR:HG22	2.13	0.49
1:A:18:LEU:H	1:A:18:LEU:CD1	2.18	0.49
1:A:327:GLU:C	1:A:329:ARG:H	2.15	0.49
1:C:265:LYS:HB2	1:C:268:TRP:CE2	2.47	0.49
1:D:188:ILE:HG22	1:D:188:ILE:O	2.13	0.49
2:A:501:NAD:N7N	1:B:159:THR:CG2	2.75	0.49
1:B:171:LEU:O	1:B:174:THR:HG22	2.13	0.49
1:C:212:ARG:HD3	2:C:501:NAD:C8A	2.43	0.49
1:A:20:VAL:HG12	1:A:21:GLU:N	2.28	0.48
1:C:328:LYS:HD2	1:C:373:LYS:O	2.13	0.48
1:B:111:LYS:O	1:B:115:ILE:HG13	2.13	0.48
1:D:57:TRP:CZ3	1:D:58:ASN:HB2	2.48	0.48
1:C:334:LYS:O	1:C:338:LEU:HG	2.14	0.48
1:D:238:PRO:C	1:D:240:ARG:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLY:HA3	2:B:501:NAD:O5B	2.14	0.48
1:B:231:GLU:N	4:B:509:HOH:O	2.46	0.48
1:D:154:ASP:O	1:D:158:GLY:N	2.46	0.48
1:D:308:HIS:CD2	1:D:308:HIS:H	2.30	0.48
1:A:32:TYR:C	1:A:36:VAL:HG12	2.34	0.48
1:C:283:ASN:HB3	2:C:501:NAD:C6N	2.39	0.48
1:A:315:LEU:HD23	1:A:359:ALA:CB	2.43	0.48
1:D:174:THR:HG23	1:D:176:LYS:CG	2.41	0.48
1:A:18:LEU:HB3	1:C:89:PHE:CD2	2.49	0.48
1:A:361:ASP:OD1	1:A:363:LYS:HB2	2.13	0.48
1:C:174:THR:HG23	1:C:176:LYS:CG	2.42	0.48
1:A:12:GLY:O	1:A:15:ARG:NH2	2.47	0.48
1:A:100:PHE:HB2	1:C:100:PHE:CZ	2.49	0.48
1:A:238:PRO:C	1:A:240:ARG:H	2.17	0.48
1:B:13:LYS:CD	1:D:31:LEU:HD22	2.44	0.47
1:B:121:PRO:O	1:D:81:LEU:HD22	2.14	0.47
1:B:135:LYS:O	1:B:139:ILE:HG13	2.14	0.47
1:B:322:MET:O	1:B:326:VAL:HG23	2.14	0.47
1:C:138:ARG:HB2	1:C:138:ARG:NH1	2.29	0.47
1:A:153:HIS:HD2	4:A:516:HOH:O	1.96	0.47
1:A:154:ASP:HB2	4:A:516:HOH:O	2.14	0.47
1:B:28:LEU:HD21	1:D:90:LEU:HD21	1.96	0.47
1:D:328:LYS:HD2	1:D:373:LYS:O	2.14	0.47
1:D:310:ASN:N	4:D:852:HOH:O	2.47	0.47
2:A:501:NAD:N7N	1:B:159:THR:OG1	2.48	0.47
1:B:138:ARG:HB2	1:B:138:ARG:CZ	2.44	0.47
1:C:156:GLN:NE2	4:C:533:HOH:O	2.47	0.47
1:A:361:ASP:HB3	1:A:364:VAL:HG23	1.96	0.47
1:C:213:LYS:HB2	1:C:223:THR:HA	1.97	0.47
1:C:361:ASP:HB3	1:C:364:VAL:HG23	1.96	0.47
1:D:254:PHE:CD2	1:D:277:VAL:HB	2.50	0.47
1:B:24:ASP:OD1	1:B:24:ASP:N	2.48	0.47
1:B:32:TYR:O	1:B:36:VAL:HG12	2.13	0.47
1:C:287:GLU:CG	4:C:535:HOH:O	2.61	0.47
1:C:238:PRO:C	1:C:240:ARG:H	2.17	0.47
1:C:347:SER:O	1:C:348:CYS:HB3	2.15	0.47
1:D:265:LYS:HB2	1:D:268:TRP:CE2	2.49	0.47
1:B:28:LEU:CD2	1:D:90:LEU:HD21	2.45	0.46
1:B:185:VAL:C	4:B:523:HOH:O	2.53	0.46
1:B:351:GLU:CG	1:B:354:ARG:HB3	2.42	0.46
1:D:219:ASN:O	1:D:221:PRO:CD	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:LYS:N	4:D:802:HOH:O	2.48	0.46
1:A:109:GLU:OE2	1:A:138:ARG:HD2	2.16	0.46
1:B:211:ASP:CG	1:B:212:ARG:H	2.17	0.46
1:C:340:ALA:O	1:C:344:ILE:HG13	2.15	0.46
1:A:283:ASN:C	1:A:283:ASN:OD1	2.53	0.46
1:C:259:SER:O	2:C:501:NAD:O3D	2.28	0.46
1:C:369:TYR:O	1:C:373:LYS:HB2	2.15	0.46
1:B:369:TYR:O	1:B:373:LYS:HB2	2.16	0.46
1:A:52:VAL:HG12	1:A:52:VAL:O	2.15	0.46
1:A:159:THR:HG21	2:B:501:NAD:N7N	2.31	0.46
1:A:213:LYS:O	1:A:223:THR:HG22	2.16	0.46
1:D:311:GLN:O	1:D:356:ILE:HD11	2.15	0.46
1:B:100:PHE:CD1	1:D:100:PHE:CD1	3.03	0.46
1:B:178:ILE:HG23	1:B:179:GLU:N	2.31	0.46
1:D:159:THR:O	1:D:163:VAL:HG23	2.16	0.46
1:D:240:ARG:NH2	4:D:806:HOH:O	2.48	0.46
1:D:314:ASN:O	1:D:317:ALA:CB	2.64	0.46
1:D:369:TYR:O	1:D:373:LYS:HB2	2.15	0.46
1:A:347:SER:O	1:A:348:CYS:HB3	2.15	0.46
1:D:154:ASP:OD2	1:D:314:ASN:HB3	2.16	0.46
1:A:211:ASP:CG	1:A:212:ARG:H	2.18	0.46
1:B:174:THR:CG2	1:B:176:LYS:H	2.28	0.46
1:D:294:ARG:HB2	4:D:809:HOH:O	2.13	0.46
1:A:92:LYS:HB3	1:C:18:LEU:HD21	1.98	0.45
1:D:361:ASP:HB3	1:D:364:VAL:HG23	1.98	0.45
1:A:16:THR:O	1:A:17:ALA:HB2	2.17	0.45
1:B:231:GLU:N	4:B:506:HOH:O	2.49	0.45
1:C:138:ARG:HB2	1:C:138:ARG:CZ	2.46	0.45
1:C:178:ILE:HG23	1:C:179:GLU:N	2.32	0.45
1:D:211:ASP:OD1	1:D:212:ARG:HG2	2.16	0.45
1:D:152:PHE:HB2	1:D:332:ILE:CD1	2.47	0.45
1:D:262:ASN:ND2	1:D:285:VAL:HG11	2.31	0.45
1:A:87:LYS:HE3	1:A:129:GLU:OE1	2.15	0.45
1:B:109:GLU:OE2	1:B:138:ARG:HD2	2.15	0.45
1:B:232:ILE:N	4:B:510:HOH:O	2.46	0.45
1:D:354:ARG:HG3	1:D:354:ARG:HH11	1.81	0.45
1:B:14:ILE:HG23	1:B:15:ARG:N	2.30	0.45
1:B:138:ARG:HB2	1:B:138:ARG:NH1	2.31	0.45
1:B:347:SER:O	1:B:348:CYS:HB3	2.16	0.45
1:D:315:LEU:C	1:D:317:ALA:H	2.20	0.45
1:B:2:ASP:OD2	1:B:5:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:SER:HB3	1:C:202:LEU:HD11	1.99	0.45
1:C:264:LEU:HD23	1:C:264:LEU:C	2.36	0.45
1:A:226:ASN:C	1:A:228:TYR:H	2.20	0.45
1:A:265:LYS:HB2	1:A:268:TRP:CE2	2.51	0.45
1:A:317:ALA:O	1:A:321:ILE:HG13	2.16	0.45
1:B:13:LYS:CG	1:D:31:LEU:HD22	2.47	0.45
1:B:361:ASP:OD1	1:B:363:LYS:HB2	2.16	0.45
1:D:56:ARG:HG2	1:D:56:ARG:HH11	1.81	0.45
1:D:69:VAL:CA	1:D:130:ASP:OD2	2.57	0.45
1:D:249:LEU:O	1:D:272:MET:HG2	2.17	0.45
1:D:322:MET:O	1:D:326:VAL:HG23	2.17	0.45
1:B:265:LYS:HB2	1:B:268:TRP:CE2	2.52	0.45
1:D:25:ARG:HG3	1:D:25:ARG:HH11	1.81	0.45
1:D:269:ILE:HB	4:D:802:HOH:O	2.16	0.45
1:C:283:ASN:HD22	2:C:501:NAD:C6N	2.30	0.45
1:D:290:PRO:HG2	1:D:308:HIS:CD2	2.51	0.45
1:B:315:LEU:HD23	1:B:359:ALA:CB	2.46	0.44
1:C:162:VAL:HG12	1:C:312:VAL:HG13	1.99	0.44
1:A:123:PHE:CE1	1:C:100:PHE:HE2	2.35	0.44
1:A:162:VAL:HG12	1:A:312:VAL:HG13	1.98	0.44
1:B:328:LYS:HG2	1:B:328:LYS:O	2.17	0.44
1:C:269:ILE:HD13	4:C:511:HOH:O	2.16	0.44
1:C:270:LYS:HG3	4:C:540:HOH:O	2.18	0.44
1:D:138:ARG:NH1	1:D:138:ARG:CB	2.80	0.44
1:C:264:LEU:HB3	1:C:288:ILE:HB	1.99	0.44
1:A:178:ILE:HG23	1:A:179:GLU:N	2.32	0.44
1:A:174:THR:CG2	1:A:176:LYS:H	2.30	0.44
1:C:56:ARG:HH11	1:C:56:ARG:HG2	1.81	0.44
1:D:347:SER:O	1:D:348:CYS:HB3	2.18	0.44
1:A:219:ASN:O	1:A:221:PRO:CD	2.65	0.44
1:C:174:THR:CG2	1:C:176:LYS:H	2.31	0.44
1:A:18:LEU:HB3	1:C:89:PHE:CE2	2.53	0.44
1:A:29:SER:HA	1:A:34:PRO:HD2	1.99	0.44
1:A:56:ARG:HG2	1:A:56:ARG:NH1	2.31	0.44
1:B:290:PRO:HG3	1:B:303:THR:CG2	2.48	0.44
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.74	0.43
1:B:123:PHE:HE1	1:D:100:PHE:CE2	2.36	0.43
1:C:213:LYS:O	1:C:223:THR:HG22	2.17	0.43
1:C:283:ASN:CB	2:C:501:NAD:H6N	2.39	0.43
1:C:337:LEU:O	1:C:341:VAL:HG23	2.18	0.43
1:D:213:LYS:O	1:D:223:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD23	1:A:359:ALA:HB1	2.01	0.43
1:B:186:ASN:C	4:B:523:HOH:O	2.56	0.43
1:B:191:ALA:O	1:B:195:ILE:HG13	2.18	0.43
1:C:252:ALA:O	1:C:272:MET:HB3	2.18	0.43
1:A:28:LEU:O	1:A:30:LEU:N	2.52	0.43
1:A:290:PRO:CG	1:A:303:THR:HG21	2.47	0.43
1:A:215:ILE:HD11	1:A:248:ALA:HB2	2.00	0.43
1:C:124:GLY:O	1:C:150:PRO:HD2	2.19	0.43
1:A:135:LYS:O	1:A:139:ILE:HG13	2.19	0.43
1:B:16:THR:O	1:B:17:ALA:HB2	2.19	0.43
1:B:361:ASP:HB3	1:B:364:VAL:HG23	2.00	0.43
1:C:286:PRO:O	1:C:287:GLU:C	2.56	0.43
1:D:160:ALA:HB1	1:D:198:PHE:CD1	2.53	0.43
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.83	0.43
1:C:55:SER:O	1:C:56:ARG:C	2.56	0.43
1:D:169:ASN:ND2	1:D:355:ILE:O	2.52	0.43
1:A:290:PRO:HG3	1:A:303:THR:CG2	2.46	0.42
1:A:351:GLU:CG	1:A:354:ARG:HB3	2.45	0.42
1:B:132:GLY:O	1:B:136:CYS:HB3	2.19	0.42
1:C:147:MET:O	1:C:331:LYS:NZ	2.52	0.42
1:A:8:ARG:HG3	1:C:52:VAL:HG13	2.01	0.42
1:C:361:ASP:OD1	1:C:363:LYS:HB2	2.18	0.42
1:B:219:ASN:O	1:B:221:PRO:CD	2.65	0.42
4:B:526:HOH:O	1:D:306:SER:HB3	2.19	0.42
1:D:315:LEU:HD23	1:D:359:ALA:CB	2.49	0.42
1:B:226:ASN:C	1:B:228:TYR:H	2.22	0.42
1:C:56:ARG:HG2	1:C:56:ARG:NH1	2.35	0.42
1:D:337:LEU:O	1:D:341:VAL:HG23	2.20	0.42
1:A:24:ASP:OD1	1:A:24:ASP:N	2.52	0.42
1:A:160:ALA:HB1	1:A:198:PHE:CD1	2.55	0.42
1:B:22:LYS:HB2	1:C:57:TRP:CH2	2.55	0.42
1:C:120:GLU:HB3	1:C:121:PRO:HD3	2.01	0.42
1:D:164:SER:HB3	1:D:202:LEU:HD11	2.02	0.42
1:D:276:PRO:HA	4:D:811:HOH:O	2.19	0.42
1:A:31:LEU:HD13	1:C:13:LYS:HG2	2.02	0.42
1:A:124:GLY:O	1:A:150:PRO:HD2	2.19	0.42
1:C:364:VAL:O	1:C:368:VAL:HG23	2.20	0.42
1:A:369:TYR:O	1:A:373:LYS:HB2	2.19	0.42
1:D:83:VAL:HB	1:D:84:MET:HE2	2.02	0.42
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.63	0.42
1:C:157:GLN:O	1:C:161:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:CD2	1:C:359:ALA:HB1	2.50	0.42
2:A:501:NAD:O2D	1:B:283:ASN:ND2	2.53	0.41
1:B:39:VAL:CG2	1:D:4:LEU:HD23	2.50	0.41
1:B:283:ASN:OD1	1:B:283:ASN:C	2.58	0.41
1:C:174:THR:HG22	1:C:176:LYS:H	1.85	0.41
1:D:129:GLU:O	1:D:131:ILE:HG13	2.20	0.41
1:A:283:ASN:HB3	2:B:501:NAD:H6N	2.02	0.41
1:D:309:PRO:O	1:D:310:ASN:C	2.58	0.41
1:D:317:ALA:O	1:D:321:ILE:HG13	2.20	0.41
1:D:364:VAL:O	1:D:368:VAL:HG23	2.19	0.41
1:B:124:GLY:O	1:B:150:PRO:HD2	2.20	0.41
1:C:226:ASN:OD1	1:C:228:TYR:HD2	2.03	0.41
1:D:252:ALA:O	1:D:272:MET:HB3	2.21	0.41
1:D:323:LYS:HG2	1:D:369:TYR:CE1	2.55	0.41
1:B:35:GLY:O	1:B:36:VAL:C	2.58	0.41
1:B:36:VAL:HG13	1:B:37:ALA:N	2.35	0.41
1:B:39:VAL:HG22	1:D:4:LEU:HD23	2.03	0.41
1:B:290:PRO:CG	1:B:303:THR:HG21	2.50	0.41
1:C:305:ARG:HB3	1:C:307:ASP:HB2	2.02	0.41
1:D:349:GLU:HA	1:D:350:PRO:HD2	1.93	0.41
1:A:32:TYR:HH	1:C:87:LYS:HE2	1.84	0.41
1:A:305:ARG:NH2	4:A:517:HOH:O	2.45	0.41
1:C:160:ALA:HB1	1:C:198:PHE:CD1	2.56	0.41
1:D:314:ASN:O	1:D:315:LEU:C	2.58	0.41
1:A:19:PRO:CG	1:A:20:VAL:H	2.32	0.41
1:B:15:ARG:HH11	1:B:15:ARG:CG	2.33	0.41
1:B:115:ILE:HG23	1:D:115:ILE:HG23	2.03	0.41
1:B:162:VAL:HG12	1:B:312:VAL:HG13	2.02	0.41
1:B:215:ILE:HD11	1:B:248:ALA:HB2	2.01	0.41
1:C:57:TRP:CD2	1:C:58:ASN:HB2	2.55	0.41
1:C:131:ILE:HG22	1:C:136:CYS:HB3	2.02	0.41
1:C:212:ARG:C	1:C:213:LYS:HD2	2.41	0.41
1:C:256:ILE:HA	1:C:279:PHE:HB2	2.02	0.41
1:D:169:ASN:HB3	1:D:350:PRO:HB3	2.03	0.41
1:D:57:TRP:CD2	1:D:58:ASN:HB2	2.55	0.41
1:A:191:ALA:O	1:A:195:ILE:HG13	2.21	0.40
1:C:20:VAL:HG12	1:C:21:GLU:N	2.35	0.40
1:D:55:SER:HB3	1:D:59:THR:HG23	2.03	0.40
1:D:315:LEU:O	1:D:319:PRO:HD2	2.20	0.40
1:A:100:PHE:HE2	1:C:123:PHE:CE1	2.39	0.40
1:C:55:SER:O	1:C:57:TRP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:THR:CG2	2:C:501:NAD:N7N	2.78	0.40
1:C:219:ASN:O	1:C:221:PRO:CD	2.66	0.40
1:C:254:PHE:CD2	1:C:277:VAL:HB	2.57	0.40
1:D:129:GLU:O	1:D:130:ASP:C	2.58	0.40
1:A:174:THR:HG23	1:A:176:LYS:CG	2.48	0.40
1:B:14:ILE:CD1	1:B:88:ALA:HB1	2.51	0.40
1:B:100:PHE:HE2	1:D:123:PHE:CE1	2.40	0.40
1:B:317:ALA:O	1:B:321:ILE:HG13	2.21	0.40
1:C:317:ALA:O	1:C:321:ILE:HG13	2.22	0.40
1:D:256:ILE:HA	1:D:279:PHE:HB2	2.02	0.40
1:D:294:ARG:HH22	1:D:309:PRO:HD2	1.87	0.40
1:B:30:LEU:O	1:D:7:HIS:HE1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	369/386 (96%)	319 (86%)	43 (12%)	7 (2%)	8 31
1	B	369/386 (96%)	318 (86%)	47 (13%)	4 (1%)	14 45
1	C	369/386 (96%)	322 (87%)	39 (11%)	8 (2%)	6 27
1	D	369/386 (96%)	314 (85%)	46 (12%)	9 (2%)	6 25
All	All	1476/1544 (96%)	1273 (86%)	175 (12%)	28 (2%)	8 31

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	LEU
1	B	225	LEU
1	C	225	LEU

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Mol	Chain	Res	Type
1	C	273	SER
1	D	225	LEU
1	D	273	SER
1	A	17	ALA
1	A	29	SER
1	A	227	GLU
1	B	227	GLU
1	C	227	GLU
1	C	309	PRO
1	D	227	GLU
1	D	310	ASN
1	A	56	ARG
1	C	310	ASN
1	C	329	ARG
1	D	45	GLU
1	D	307	ASP
1	C	21	GLU
1	D	309	PRO
1	A	25	ARG
1	B	25	ARG
1	C	56	ARG
1	B	220	ASP
1	A	220	ASP
1	D	258	VAL
1	D	220	ASP

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	309/321 (96%)	294 (95%)	15 (5%)	25	56
1	B	309/321 (96%)	295 (96%)	14 (4%)	27	59
1	C	309/321 (96%)	296 (96%)	13 (4%)	30	60
1	D	309/321 (96%)	293 (95%)	16 (5%)	23	53
All	All	1236/1284 (96%)	1178 (95%)	58 (5%)	26	57

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	18	LEU
1	A	23	VAL
1	A	25	ARG
1	A	41	ARG
1	A	127	ASN
1	A	154	ASP
1	A	174	THR
1	A	179	GLU
1	A	218	GLU
1	A	274	ARG
1	A	283	ASN
1	A	307	ASP
1	A	314	ASN
1	A	335	ASN
1	B	6	LEU
1	B	14	ILE
1	B	18	LEU
1	B	127	ASN
1	B	154	ASP
1	B	174	THR
1	B	179	GLU
1	B	218	GLU
1	B	274	ARG
1	B	283	ASN
1	B	307	ASP
1	B	314	ASN
1	B	335	ASN
1	B	352	PRO
1	C	6	LEU
1	C	25	ARG
1	C	45	GLU
1	C	127	ASN
1	C	154	ASP
1	C	174	THR
1	C	179	GLU
1	C	218	GLU
1	C	274	ARG
1	C	283	ASN
1	C	314	ASN
1	C	335	ASN
1	C	370	THR

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Mol	Chain	Res	Type
1	D	14	ILE
1	D	15	ARG
1	D	18	LEU
1	D	87	LYS
1	D	127	ASN
1	D	130	ASP
1	D	154	ASP
1	D	155	ASP
1	D	174	THR
1	D	179	GLU
1	D	218	GLU
1	D	274	ARG
1	D	283	ASN
1	D	314	ASN
1	D	335	ASN
1	D	352	PRO

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	127	ASN
1	A	148	ASN
1	A	186	ASN
1	A	283	ASN
1	A	335	ASN
1	B	127	ASN
1	B	148	ASN
1	B	186	ASN
1	B	283	ASN
1	B	314	ASN
1	B	335	ASN
1	C	127	ASN
1	C	148	ASN
1	C	186	ASN
1	C	194	ASN
1	C	262	ASN
1	C	308	HIS
1	C	335	ASN
1	D	7	HIS
1	D	127	ASN
1	D	148	ASN
1	D	186	ASN

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Mol	Chain	Res	Type
1	D	194	ASN
1	D	262	ASN
1	D	308	HIS
1	D	311	GLN
1	D	335	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	NAD	B	501	-	42,48,48	2.02	8 (19%)	50,73,73	1.85	11 (22%)
2	NAD	A	501	-	42,48,48	2.04	8 (19%)	50,73,73	1.88	11 (22%)
2	NAD	C	501	-	42,48,48	2.04	8 (19%)	50,73,73	1.85	11 (22%)

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	B	501	-	-	5/26/62/62	0/5/5/5
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
2	NAD	C	501	-	-	3/26/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O7N-C7N	8.50	1.40	1.24
2	A	501	NAD	O7N-C7N	8.48	1.40	1.24
2	C	501	NAD	O7N-C7N	8.42	1.40	1.24
2	B	501	NAD	C2A-N3A	5.24	1.40	1.32
2	A	501	NAD	C2A-N3A	4.54	1.39	1.32
2	C	501	NAD	C2A-N1A	4.26	1.41	1.33
2	A	501	NAD	C2N-N1N	4.17	1.40	1.35
2	C	501	NAD	C2N-N1N	3.93	1.39	1.35
2	C	501	NAD	C2A-N3A	3.93	1.38	1.32
2	B	501	NAD	C2N-N1N	3.72	1.39	1.35
2	A	501	NAD	C2A-N1A	3.53	1.40	1.33
2	B	501	NAD	C2A-N1A	3.44	1.40	1.33
2	A	501	NAD	C4N-C3N	2.80	1.44	1.39
2	C	501	NAD	C6N-N1N	2.70	1.42	1.35
2	C	501	NAD	C4A-N3A	2.54	1.39	1.35
2	C	501	NAD	C2N-C3N	2.50	1.42	1.39
2	C	501	NAD	C4N-C3N	2.49	1.43	1.39
2	B	501	NAD	C6N-N1N	2.40	1.41	1.35
2	A	501	NAD	C3N-C7N	-2.36	1.47	1.50
2	A	501	NAD	C6N-N1N	2.32	1.41	1.35
2	B	501	NAD	C4N-C3N	2.31	1.43	1.39
2	B	501	NAD	C3N-C7N	-2.26	1.47	1.50
2	B	501	NAD	O4B-C4B	-2.02	1.40	1.45
2	A	501	NAD	C2N-C3N	2.02	1.42	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NAD	O2N-PN-O5D	-5.73	81.14	107.75
2	B	501	NAD	O2N-PN-O5D	-5.57	81.88	107.75
2	A	501	NAD	O2N-PN-O5D	-5.53	82.08	107.75
2	C	501	NAD	O5D-PN-O1N	-5.32	88.27	109.07
2	B	501	NAD	O5D-PN-O1N	-5.22	88.67	109.07
2	A	501	NAD	O5D-PN-O1N	-5.14	89.00	109.07
2	A	501	NAD	N3A-C2A-N1A	-5.05	120.78	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAD	N3A-C2A-N1A	-5.02	120.83	128.68
2	C	501	NAD	N3A-C2A-N1A	-4.99	120.88	128.68
2	C	501	NAD	C3N-C7N-N7N	3.72	122.21	117.75
2	B	501	NAD	C3D-C2D-C1D	-3.45	95.79	100.98
2	A	501	NAD	O4D-C1D-C2D	-3.40	101.96	106.93
2	A	501	NAD	C3D-C2D-C1D	-3.37	95.91	100.98
2	B	501	NAD	O4B-C1B-C2B	-3.21	102.24	106.93
2	A	501	NAD	C3N-C7N-N7N	3.14	121.52	117.75
2	C	501	NAD	C4A-C5A-N7A	-3.01	106.27	109.40
2	B	501	NAD	O4D-C1D-C2D	-2.92	102.66	106.93
2	A	501	NAD	C4A-C5A-N7A	-2.88	106.39	109.40
2	B	501	NAD	C3N-C7N-N7N	2.84	121.16	117.75
2	A	501	NAD	O4B-C1B-C2B	-2.84	102.78	106.93
2	C	501	NAD	C1B-N9A-C4A	-2.82	121.69	126.64
2	C	501	NAD	O4D-C1D-C2D	-2.39	103.43	106.93
2	B	501	NAD	O2D-C2D-C1D	2.36	119.58	110.85
2	B	501	NAD	C4A-C5A-N7A	-2.35	106.95	109.40
2	A	501	NAD	C3N-C2N-N1N	-2.29	118.19	120.43
2	C	501	NAD	O2N-PN-O1N	2.27	123.46	112.24
2	A	501	NAD	C2N-C3N-C4N	2.24	120.80	118.26
2	A	501	NAD	O2D-C2D-C1D	2.21	119.02	110.85
2	C	501	NAD	PN-O3-PA	-2.20	125.28	132.83
2	B	501	NAD	C2N-C3N-C4N	2.11	120.66	118.26
2	C	501	NAD	O4B-C1B-C2B	-2.09	103.88	106.93
2	B	501	NAD	C3N-C2N-N1N	-2.07	118.40	120.43
2	C	501	NAD	O7N-C7N-N7N	-2.00	119.73	122.58

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	A	501	NAD	PN-O3-PA-O1A
2	B	501	NAD	PN-O3-PA-O1A
2	C	501	NAD	C3D-C4D-C5D-O5D
2	C	501	NAD	PA-O3-PN-O1N
2	A	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	501	NAD	PA-O3-PN-O1N
2	B	501	NAD	PA-O3-PN-O1N

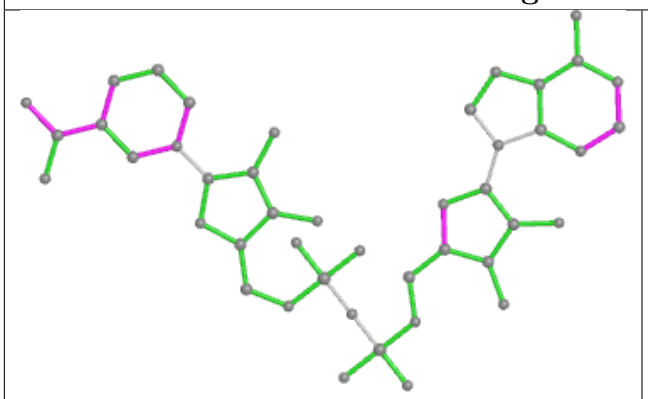
There are no ring outliers.

3 monomers are involved in 35 short contacts:

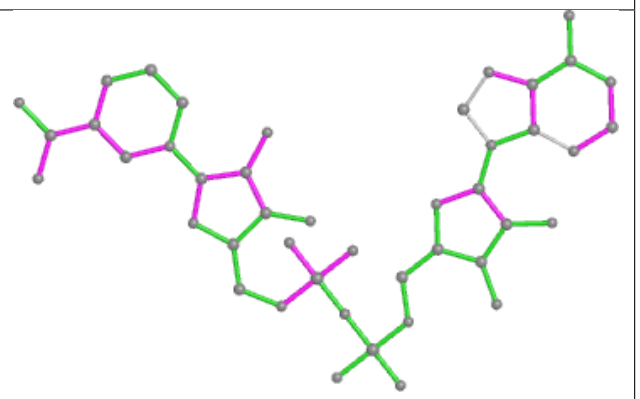
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAD	13	0
2	A	501	NAD	10	0
2	C	501	NAD	12	0

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.

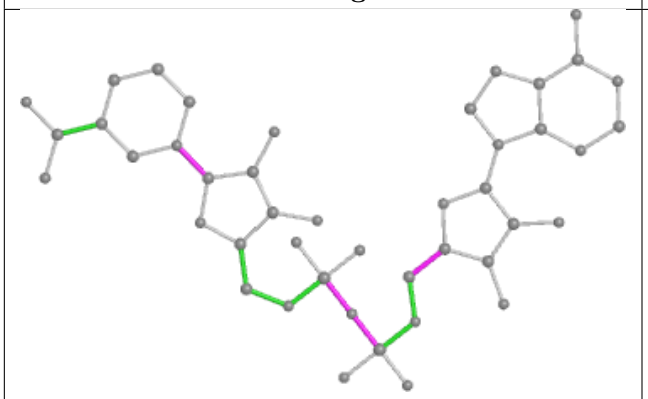
Ligand NAD B 501



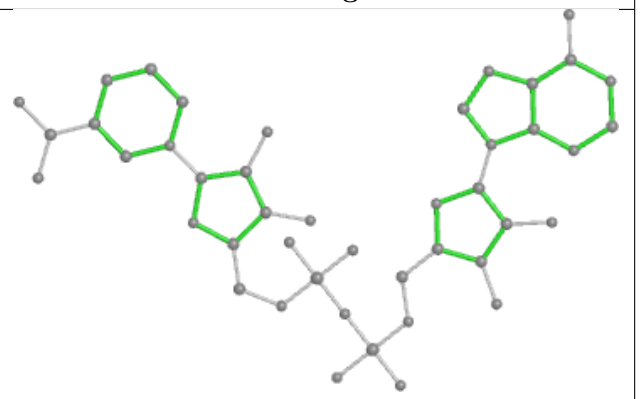
Bond lengths



Bond angles

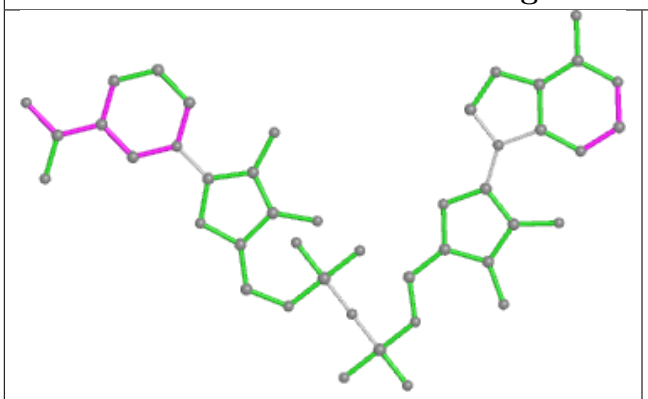


Torsions

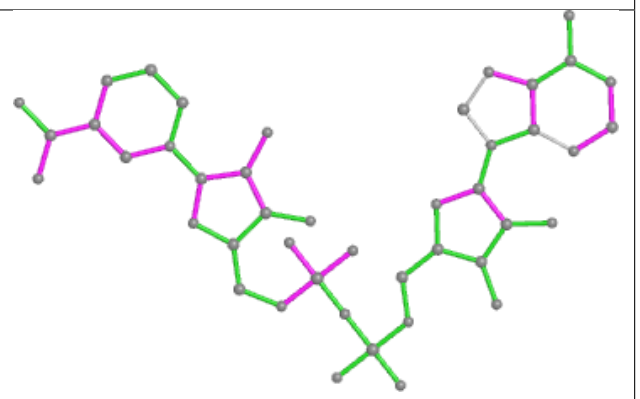


Rings

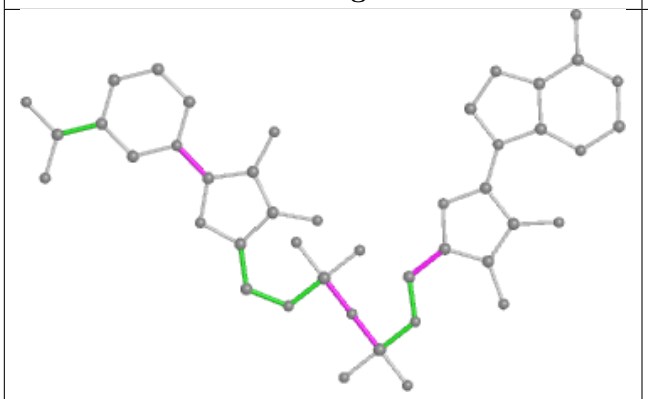
Ligand NAD A 501



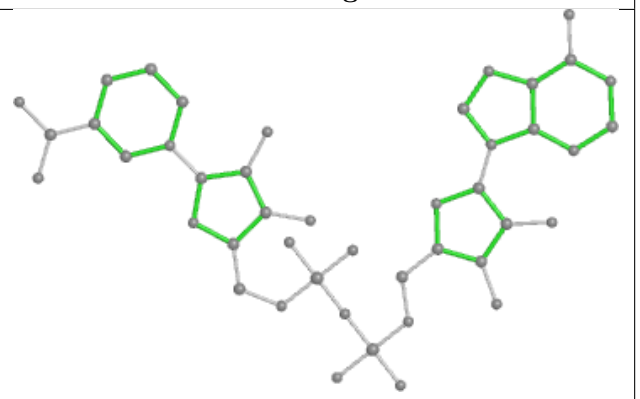
Bond lengths



Bond angles

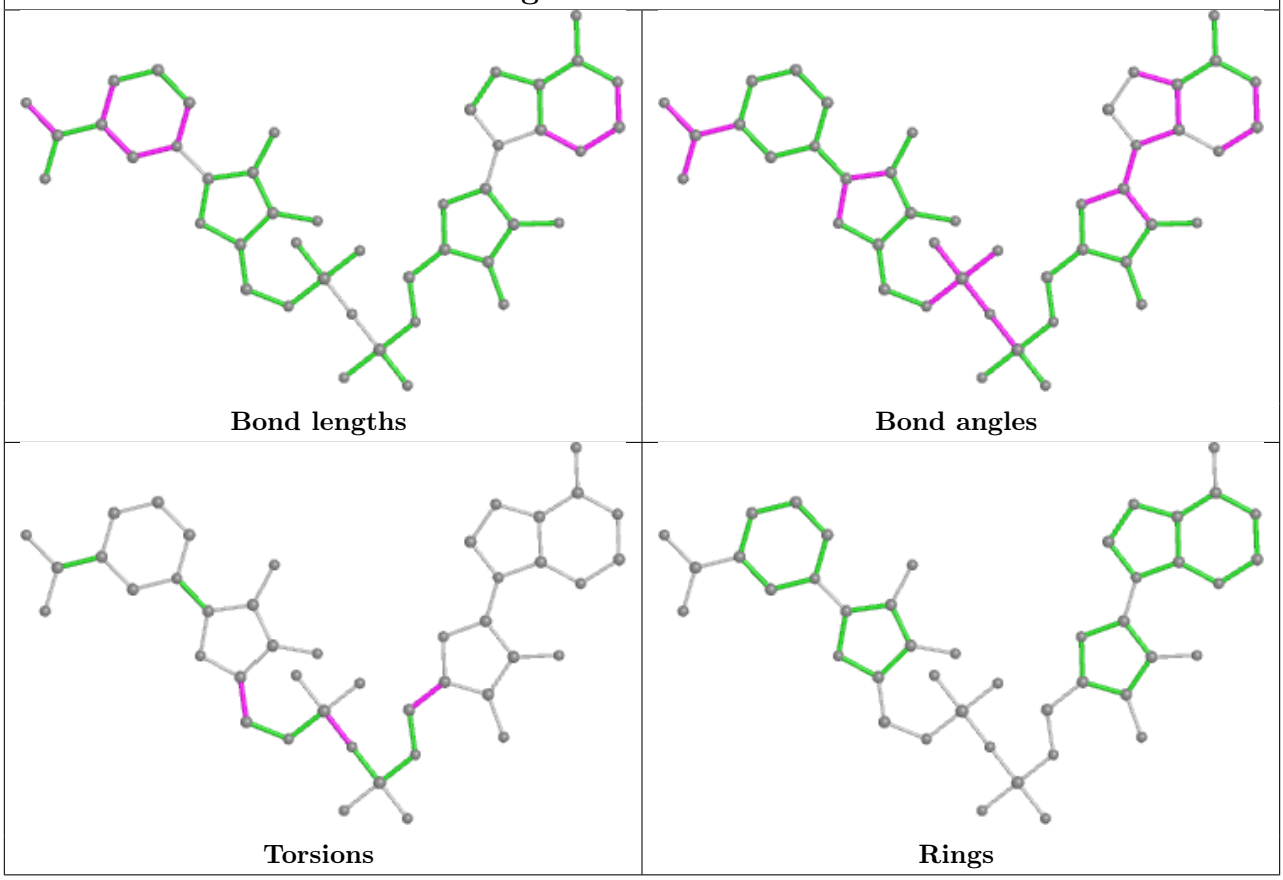


Torsions



Rings

Ligand NAD C 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	373/386 (96%)	-0.14	2 (0%)	91	83	24, 51, 66, 75	2 (0%)
1	B	373/386 (96%)	-0.12	1 (0%)	94	89	24, 52, 66, 75	2 (0%)
1	C	373/386 (96%)	0.19	23 (6%)	20	9	23, 54, 67, 77	2 (0%)
1	D	373/386 (96%)	0.01	12 (3%)	47	26	23, 54, 67, 76	2 (0%)
All	All	1492/1544 (96%)	-0.02	38 (2%)	57	37	23, 53, 67, 77	8 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	269	ILE	4.1
1	C	296	ALA	3.4
1	C	270	LYS	3.4
1	C	297	GLY	3.4
1	A	376	ALA	3.3
1	C	298	ALA	3.3
1	C	299	PHE	3.2
1	C	276	PRO	3.0
1	C	376	ALA	2.9
1	C	302	ALA	2.9
1	C	277	VAL	2.8
1	D	297	GLY	2.7
1	C	301	VAL	2.7
1	C	300	ILE	2.6
1	C	290	PRO	2.5
1	D	300	ILE	2.5
1	D	100	PHE	2.5
1	D	293	ALA	2.5
1	B	376	ALA	2.4
1	C	171	LEU	2.4
1	A	100	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	290	PRO	2.3
1	D	276	PRO	2.3
1	C	352	PRO	2.3
1	D	352	PRO	2.2
1	C	175	GLU	2.2
1	C	353	GLU	2.2
1	C	275	LYS	2.2
1	D	272	MET	2.1
1	C	173	LEU	2.1
1	D	292	LEU	2.1
1	C	177	LYS	2.1
1	D	294	ARG	2.1
1	C	278	ILE	2.1
1	D	274	ARG	2.1
1	C	260	ARG	2.0
1	D	254	PHE	2.0
1	C	355	ILE	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

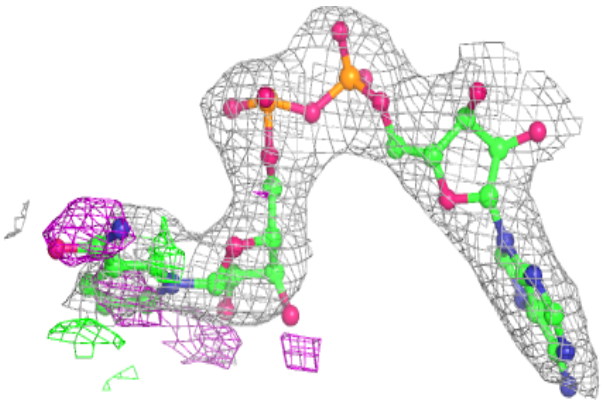
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	501	44/44	0.88	0.26	53,55,64,67	0
2	NAD	B	501	44/44	0.88	0.26	52,56,64,68	0
2	NAD	C	501	44/44	0.88	0.35	54,56,65,66	0
3	ZN	D	800	1/1	0.92	0.10	20,20,20,20	0

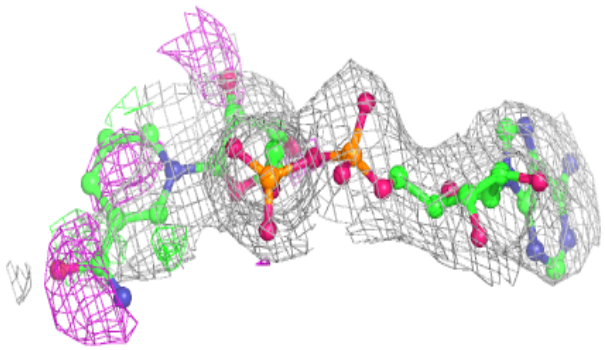
The following is a graphical depiction of the model fit to experimental electron density of all

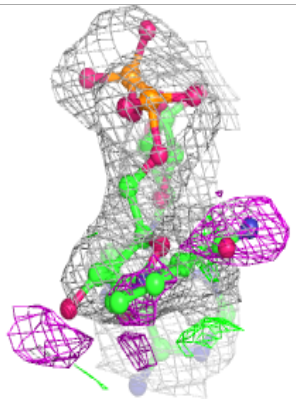
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD A 501:

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

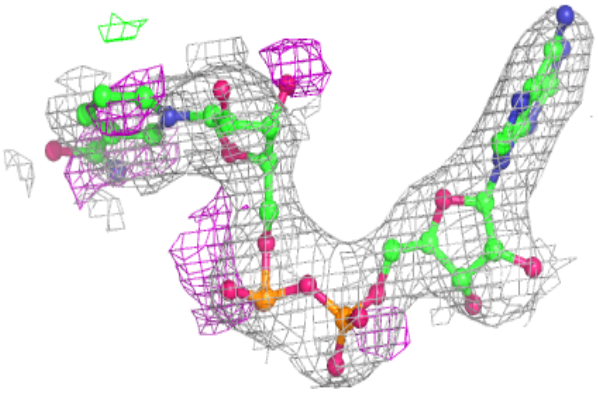


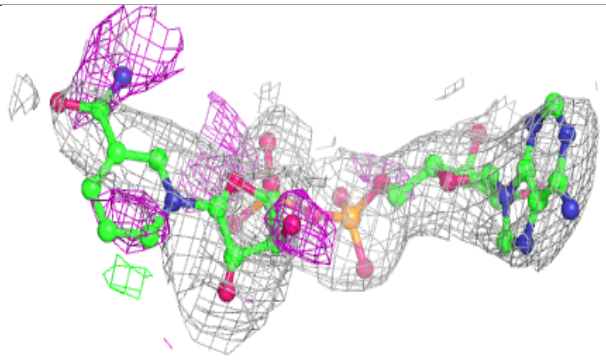


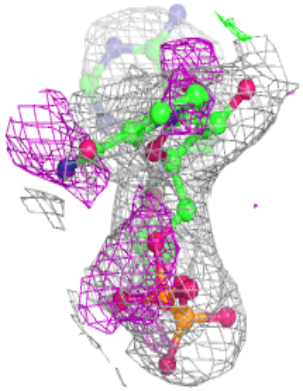


Electron density around NAD B 501:

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

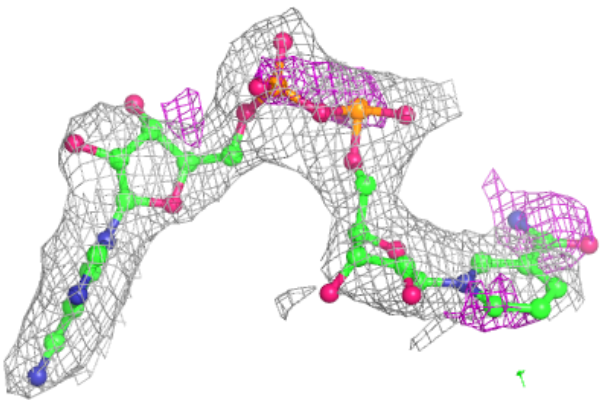


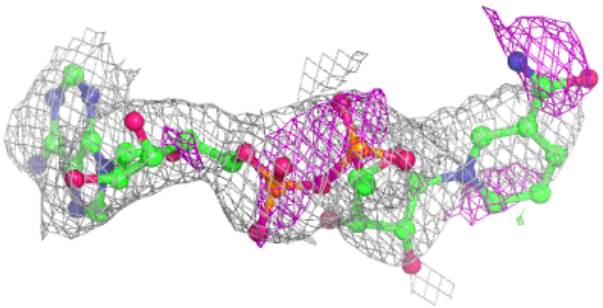


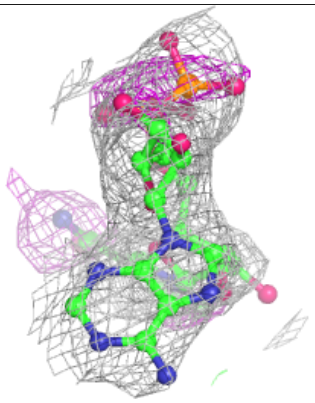


Electron density around NAD C 501:

$2mF_o$-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.