Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:37 am BST

PDB ID	:	2H5L
Title	:	S-Adenosylhomocysteine hydrolase containing NAD and 3-deaza-D-eritadeni ne
Authors	:	Yamada, T.; Komoto, J.; Takusagawa, F.
Deposited on	:	2006-05-26
Resolution	:	2.80 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:

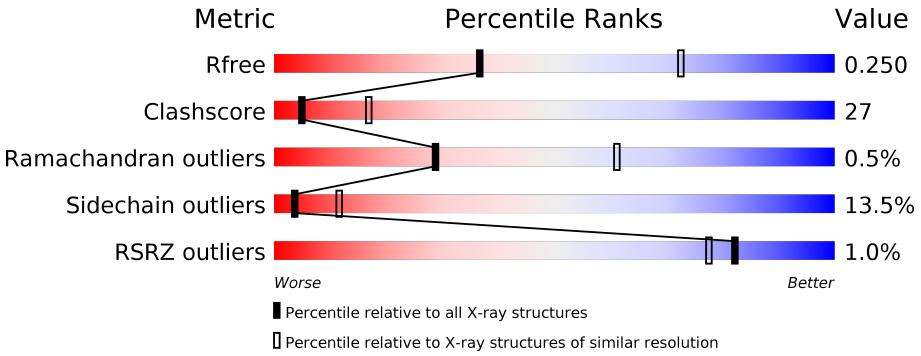
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	431	58% 35% 7%
1	B	431	% 55% 38% 7%
1	C	431	% 55% 38% 7%
1	D	431	4% 55% 38% 7%
1	E	431	% 55% 37% 7%
1	F	431	56% 36% 7%

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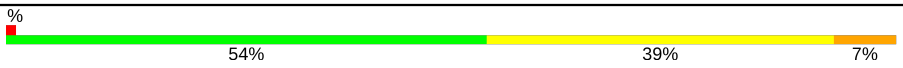
Mol	Chain	Length	Quality of chain
1	G	431	
1	H	431	

2 Entry composition (i)

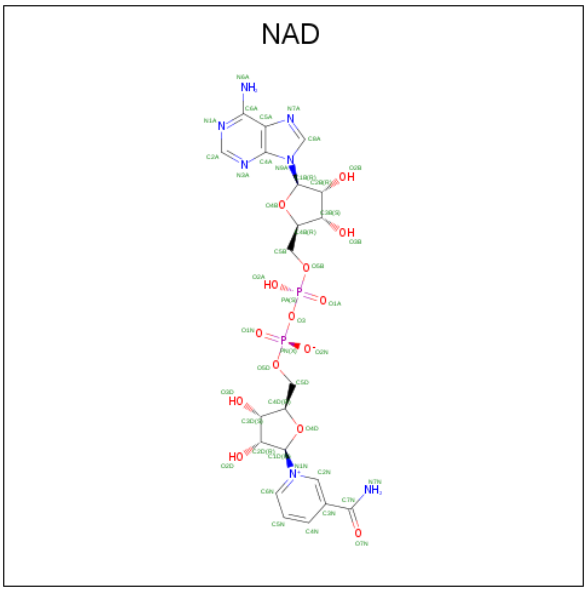
There are 4 unique types of molecules in this entry. The entry contains 27338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosylhomocysteinase.

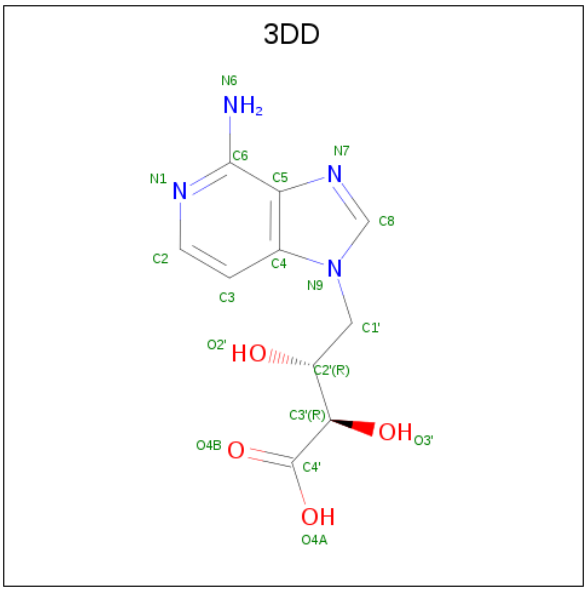
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	B	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	C	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	D	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	E	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	F	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	G	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	H	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			

- 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 (2R,3R)-4-(4-AMINO-1H-IMIDAZO[4,5-C]PYRIDIN-1-YL)-2,3-DIHYDROXYBUTANOIC ACID (three-letter code: 3DD) (formula: $C_{10}H_{12}N_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 18 10 4 4	0	0
3	B	1	Total C N O 18 10 4 4	0	0
3	C	1	Total C N O 18 10 4 4	0	0
3	D	1	Total C N O 18 10 4 4	0	0
3	E	1	Total C N O 18 10 4 4	0	0
3	F	1	Total C N O 18 10 4 4	0	0
3	G	1	Total C N O 18 10 4 4	0	0
3	H	1	Total C N O 18 10 4 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	47	Total O 47 47	0	0
4	B	30	Total O 30 30	0	0
4	C	28	Total O 28 28	0	0
4	D	34	Total O 34 34	0	0

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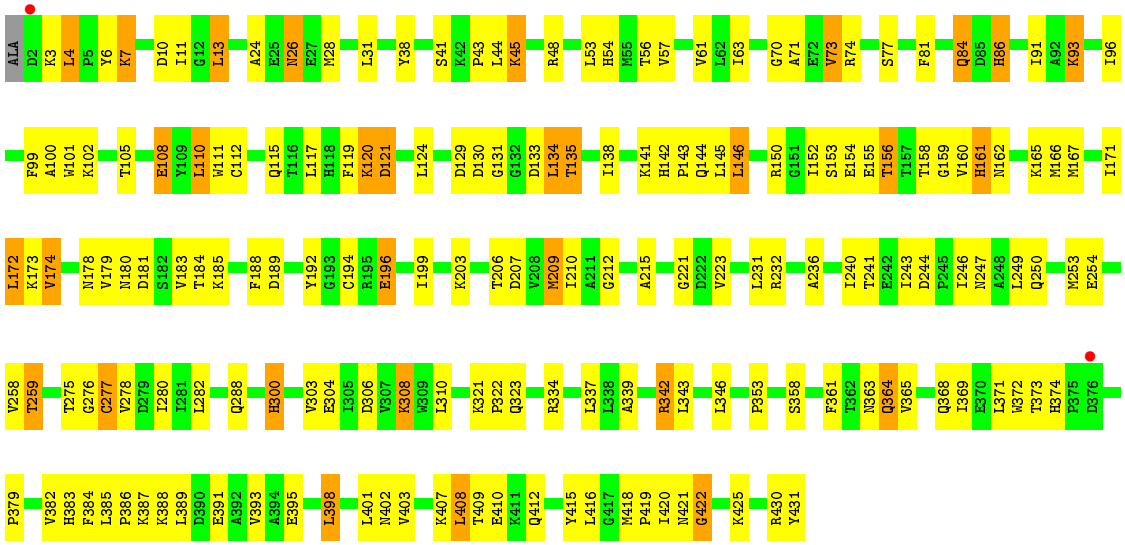
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	53	Total O 53 53	0	0
4	F	35	Total O 35 35	0	0
4	G	33	Total O 33 33	0	0
4	H	30	Total O 30 30	0	0

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.

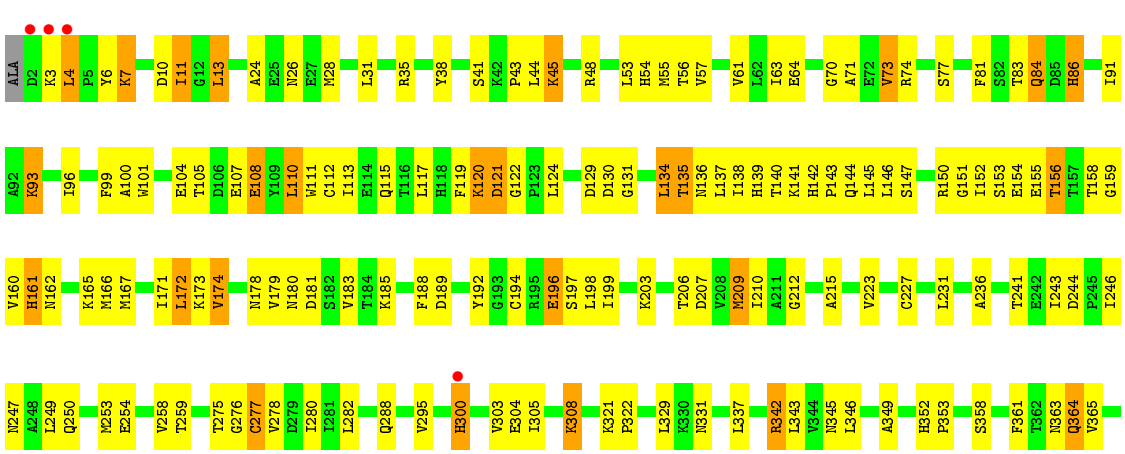
- Molecule 1: Adenosylhomocysteinase

Chain A:



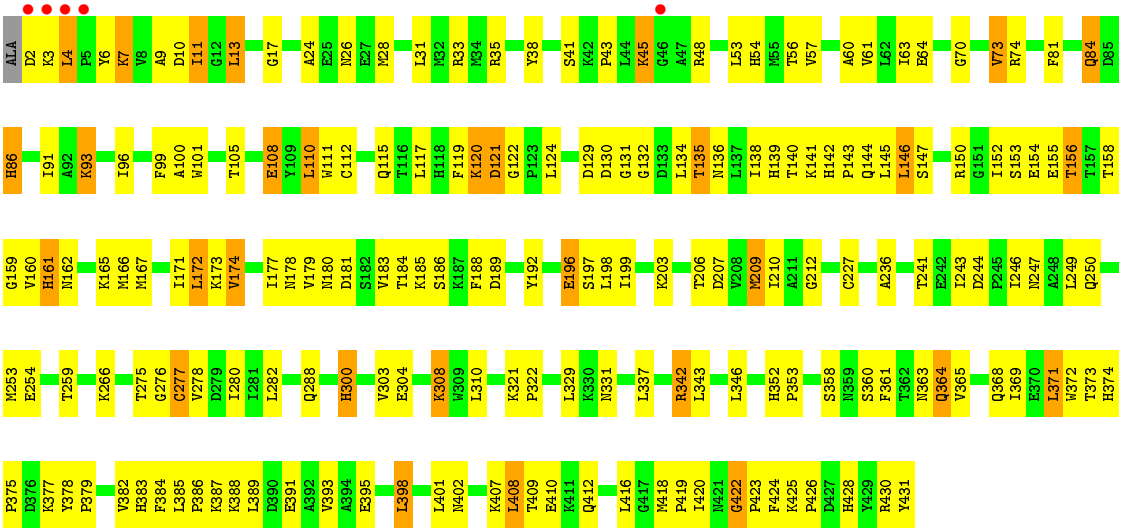
- Molecule 1: Adenosylhomocysteinase

Chain B:



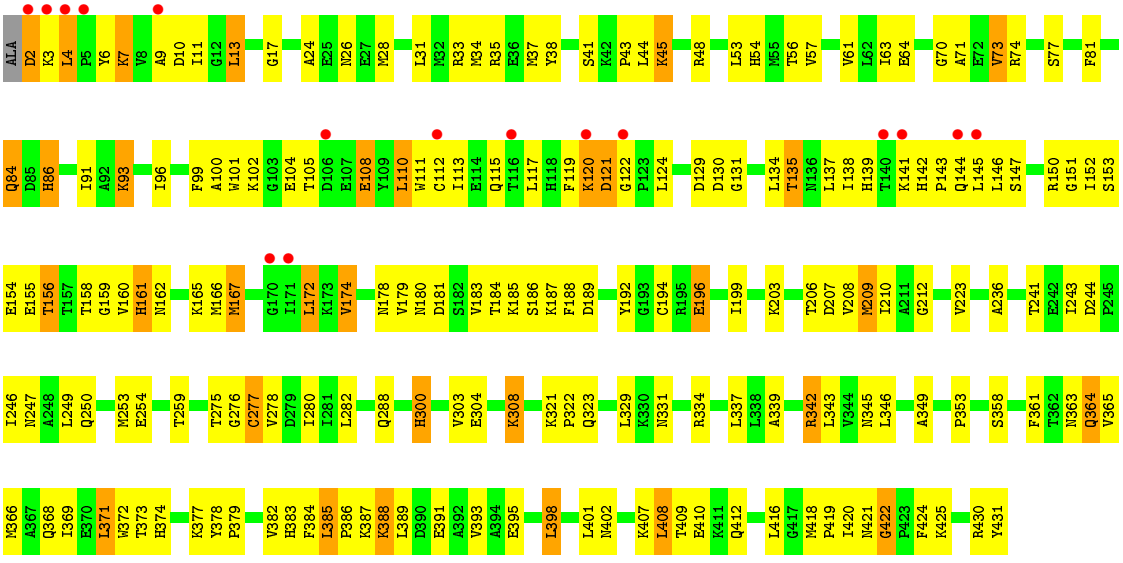
- Molecule 1: Adenosylhomocysteinase

Chain C:



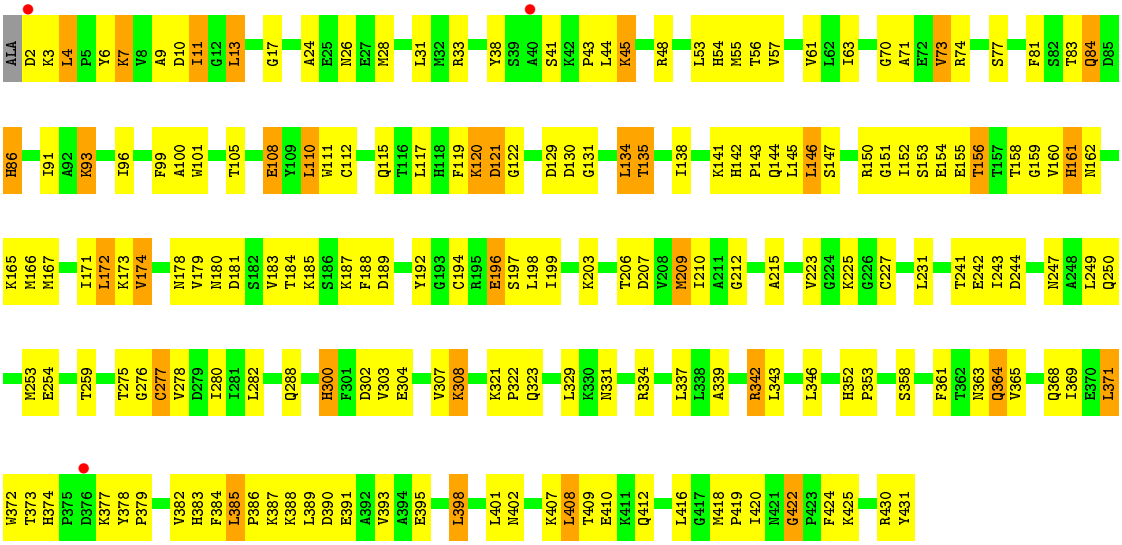
- Molecule 1: Adenosylhomocysteinase

Chain D:



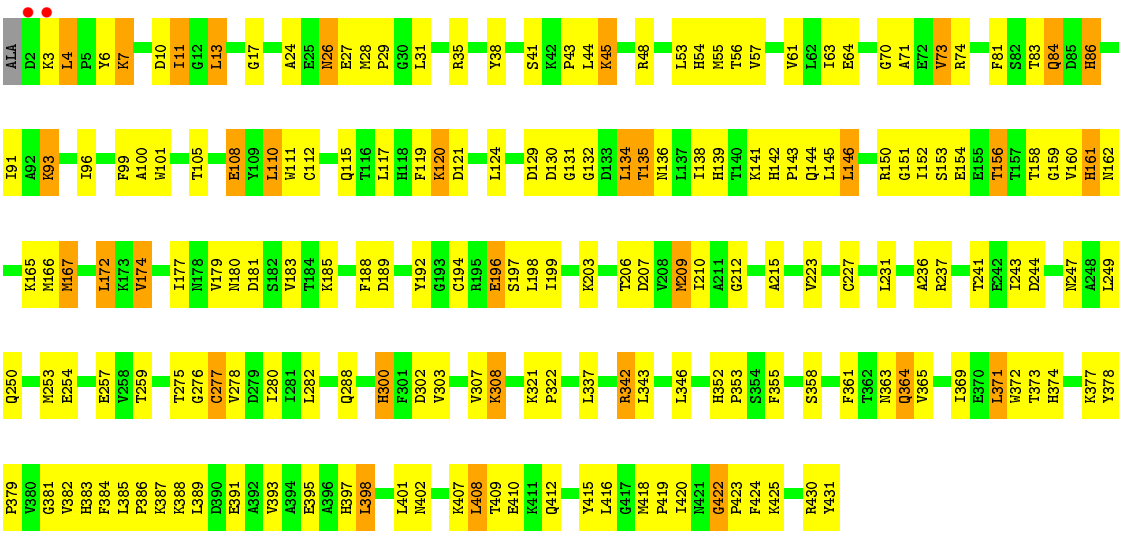
- Molecule 1: Adenosylhomocysteinase

Chain E:



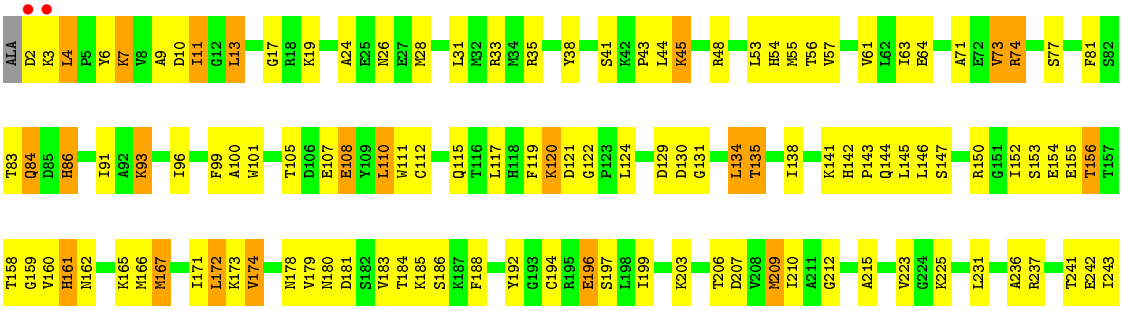
• Molecule 1: Adenosylhomocysteinase

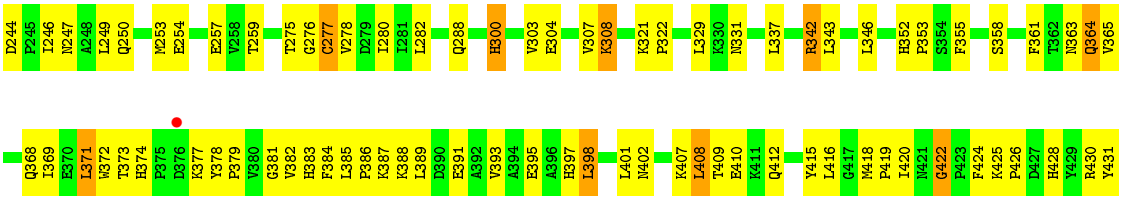
Chain F:



• Molecule 1: Adenosylhomocysteinase

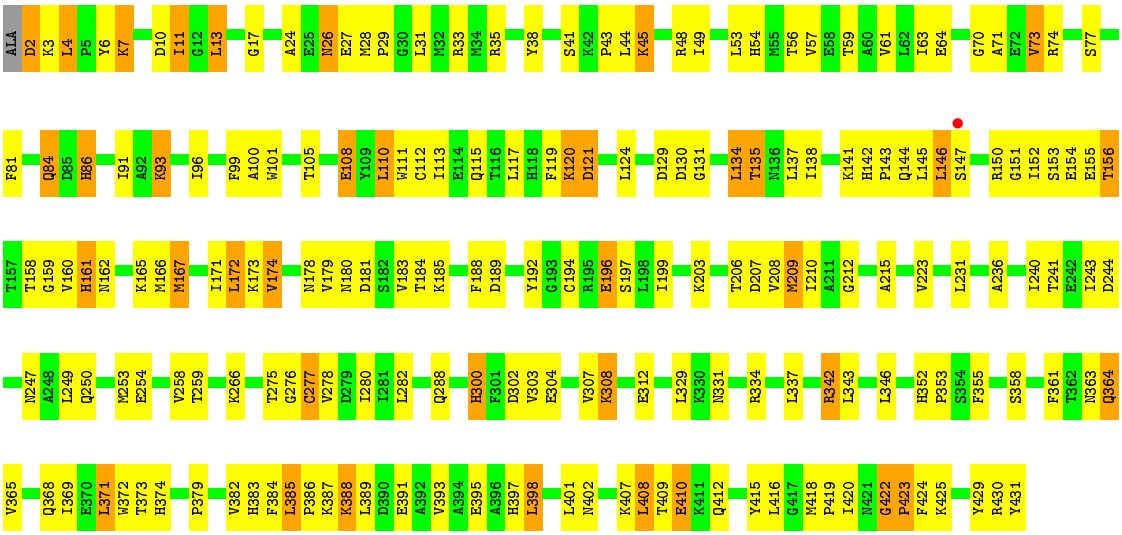
Chain G:





- Molecule 1: Adenosylhomocysteinase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.50Å 178.60Å 112.66Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 91.92 – 2.78	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 92.3 (91.92-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.77Å)	Xtriage
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.248 , 0.283 0.221 , 0.250	Depositor DCC
R_{free} test set	7944 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 10.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	27338	wwPDB-VP
Average B, all atoms (Å^2)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.76% 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: 3DD, 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	0.39	0/3384	0.60	0/4579
1	B	0.39	0/3384	0.60	0/4579
1	C	0.39	0/3384	0.61	0/4579
1	D	0.40	0/3384	0.61	0/4579
1	E	0.38	0/3384	0.61	0/4579
1	F	0.39	0/3384	0.61	0/4579
1	G	0.38	0/3384	0.61	0/4579
1	H	0.38	0/3384	0.61	0/4579
All	All	0.39	0/27072	0.61	0/36632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3319	0	3341	193	0
1	B	3319	0	3341	205	0
1	C	3319	0	3341	198	0
1	D	3319	0	3341	207	0
1	E	3319	0	3341	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3319	0	3341	187	0
1	G	3319	0	3341	200	0
1	H	3319	0	3341	199	0
2	A	44	0	26	6	0
2	B	44	0	26	5	0
2	C	44	0	26	6	0
2	D	44	0	26	6	0
2	E	44	0	26	6	0
2	F	44	0	26	5	0
2	G	44	0	26	5	0
2	H	44	0	26	4	0
3	A	18	0	11	0	0
3	B	18	0	11	0	0
3	C	18	0	11	0	0
3	D	18	0	11	0	0
3	E	18	0	11	0	0
3	F	18	0	11	0	0
3	G	18	0	11	0	0
3	H	18	0	11	0	0
4	A	47	0	0	2	0
4	B	30	0	0	1	0
4	C	28	0	0	2	0
4	D	34	0	0	10	0
4	E	53	0	0	1	0
4	F	35	0	0	1	0
4	G	33	0	0	3	0
4	H	30	0	0	2	0
All	All	27338	0	27024	1480	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (1480) 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:G:105:THR:H	1:G:108:GLU:HG3	1.18	1.08
1:F:275:THR:HG22	1:F:277:CYS:H	1.18	1.08
1:B:275:THR:HG22	1:B:277:CYS:H	1.16	1.08
1:E:275:THR:HG22	1:E:277:CYS:H	1.13	1.07
1:C:275:THR:HG22	1:C:277:CYS:H	1.17	1.07
1:D:105:THR:H	1:D:108:GLU:HG3	1.17	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:275:THR:HG22	1:H:277:CYS:H	1.18	1.07
1:G:275:THR:HG22	1:G:277:CYS:H	1.16	1.06
1:C:105:THR:H	1:C:108:GLU:HG3	1.21	1.05
1:B:105:THR:H	1:B:108:GLU:HG3	1.16	1.05
1:D:275:THR:HG22	1:D:277:CYS:H	1.19	1.04
1:A:275:THR:HG22	1:A:277:CYS:H	1.20	1.04
1:A:105:THR:H	1:A:108:GLU:HG3	1.22	1.03
1:A:7:LYS:HZ3	1:A:101:TRP:HE3	1.06	1.03
1:E:105:THR:H	1:E:108:GLU:HG3	1.23	1.02
1:F:105:THR:H	1:F:108:GLU:HG3	1.22	1.01
1:C:7:LYS:HZ3	1:C:101:TRP:HE3	1.07	0.97
1:H:105:THR:H	1:H:108:GLU:HG3	1.26	0.97
1:D:7:LYS:HZ3	1:D:101:TRP:HE3	1.09	0.96
1:G:7:LYS:HZ3	1:G:101:TRP:HE3	1.09	0.95
1:B:7:LYS:HZ3	1:B:101:TRP:HE3	1.04	0.95
1:B:156:THR:HG23	1:B:159:GLY:H	1.32	0.94
1:G:156:THR:HG23	1:G:159:GLY:H	1.31	0.94
1:D:156:THR:HG23	1:D:159:GLY:H	1.32	0.94
1:H:156:THR:HG23	1:H:159:GLY:H	1.32	0.93
1:E:156:THR:HG23	1:E:159:GLY:H	1.32	0.93
1:D:300:HIS:H	2:D:432:NAD:H1D	1.34	0.92
1:C:156:THR:HG23	1:C:159:GLY:H	1.33	0.92
1:F:156:THR:HG23	1:F:159:GLY:H	1.32	0.92
1:A:300:HIS:H	2:A:432:NAD:H1D	1.33	0.92
1:H:7:LYS:HZ3	1:H:101:TRP:HE3	1.12	0.92
1:A:156:THR:HG23	1:A:159:GLY:H	1.32	0.92
1:F:7:LYS:HZ3	1:F:101:TRP:HE3	1.08	0.92
1:H:300:HIS:H	2:H:432:NAD:H1D	1.33	0.91
1:A:308:LYS:HD2	1:A:308:LYS:H	1.36	0.90
1:E:7:LYS:HZ3	1:E:101:TRP:HE3	1.13	0.90
1:C:300:HIS:H	2:C:432:NAD:H1D	1.36	0.90
1:G:300:HIS:H	2:G:432:NAD:H1D	1.34	0.90
1:E:308:LYS:HD2	1:E:308:LYS:H	1.36	0.89
1:F:300:HIS:H	2:F:432:NAD:H1D	1.35	0.89
1:A:416:LEU:HD21	1:B:277:CYS:HB3	1.56	0.88
1:E:300:HIS:H	2:E:432:NAD:H1D	1.37	0.87
1:C:308:LYS:HD2	1:C:308:LYS:H	1.39	0.87
1:H:369:ILE:O	1:H:373:THR:HB	1.74	0.87
1:B:300:HIS:H	2:B:432:NAD:H1D	1.37	0.87
1:G:308:LYS:H	1:G:308:LYS:HD2	1.39	0.86
1:A:369:ILE:O	1:A:373:THR:HB	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:ILE:O	1:E:373:THR:HB	1.75	0.86
1:D:308:LYS:HD2	1:D:308:LYS:H	1.38	0.85
1:B:308:LYS:HD2	1:B:308:LYS:H	1.39	0.85
1:D:186:SER:HB3	4:D:434:HOH:O	1.77	0.84
1:G:180:ASN:HA	1:G:185:LYS:HD2	1.60	0.84
1:D:369:ILE:O	1:D:373:THR:HB	1.78	0.84
1:H:308:LYS:HD2	1:H:308:LYS:H	1.43	0.83
1:F:308:LYS:H	1:F:308:LYS:HD2	1.43	0.83
1:F:369:ILE:O	1:F:373:THR:HB	1.78	0.83
1:C:369:ILE:O	1:C:373:THR:HB	1.78	0.83
1:G:369:ILE:O	1:G:373:THR:HB	1.79	0.83
1:B:369:ILE:O	1:B:373:THR:HB	1.79	0.82
1:F:401:LEU:HD22	1:H:212:GLY:O	1.80	0.82
1:B:180:ASN:HA	1:B:185:LYS:HD2	1.61	0.81
1:B:7:LYS:HE2	1:B:112:CYS:SG	2.20	0.81
1:H:156:THR:CG2	1:H:159:GLY:H	1.94	0.81
1:B:156:THR:CG2	1:B:159:GLY:H	1.94	0.80
1:E:156:THR:CG2	1:E:159:GLY:H	1.94	0.80
1:A:408:LEU:HD13	1:B:243:ILE:HG21	1.63	0.79
1:E:120:LYS:HE2	1:E:120:LYS:H	1.48	0.79
1:C:275:THR:HG22	1:C:277:CYS:N	1.97	0.79
1:D:373:THR:HG21	4:D:455:HOH:O	1.83	0.79
1:G:275:THR:HG22	1:G:277:CYS:N	1.96	0.79
1:D:119:PHE:HB3	4:D:454:HOH:O	1.83	0.79
1:F:409:THR:H	1:F:412:GLN:HE21	1.30	0.78
1:D:180:ASN:HA	1:D:185:LYS:HD2	1.64	0.78
1:D:156:THR:CG2	1:D:159:GLY:H	1.96	0.78
1:E:275:THR:HG22	1:E:277:CYS:N	1.95	0.78
1:H:7:LYS:HE3	1:H:99:PHE:HB3	1.65	0.78
1:A:156:THR:CG2	1:A:159:GLY:H	1.96	0.78
1:D:409:THR:H	1:D:412:GLN:HE21	1.30	0.78
1:G:409:THR:H	1:G:412:GLN:HE21	1.31	0.78
1:C:156:THR:CG2	1:C:159:GLY:H	1.96	0.77
1:E:7:LYS:HE3	1:E:99:PHE:HB3	1.66	0.77
1:C:409:THR:H	1:C:412:GLN:HE21	1.33	0.77
1:E:277:CYS:HB3	1:F:416:LEU:HD21	1.66	0.77
1:H:409:THR:H	1:H:412:GLN:HE21	1.33	0.77
1:H:410:GLU:HG2	4:H:438:HOH:O	1.85	0.77
1:A:409:THR:H	1:A:412:GLN:HE21	1.32	0.77
1:D:120:LYS:H	1:D:120:LYS:HE2	1.48	0.76
1:B:409:THR:H	1:B:412:GLN:HE21	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:GLY:O	1:G:401:LEU:HD22	1.85	0.76
1:G:120:LYS:H	1:G:120:LYS:HE2	1.49	0.76
1:B:275:THR:HG22	1:B:277:CYS:N	1.97	0.76
1:E:243:ILE:HG21	1:F:408:LEU:HD13	1.68	0.76
1:C:419:PRO:HG2	1:C:422:GLY:HA3	1.68	0.76
1:H:275:THR:HG22	1:H:277:CYS:N	1.99	0.76
1:G:371:LEU:HD11	4:G:463:HOH:O	1.86	0.76
1:F:156:THR:CG2	1:F:159:GLY:H	1.99	0.75
1:F:353:PRO:HB2	1:H:209:MET:HB2	1.69	0.75
1:A:196:GLU:HG2	1:C:203:LYS:NZ	2.01	0.75
1:E:180:ASN:HA	1:E:185:LYS:HD2	1.68	0.75
1:E:409:THR:H	1:E:412:GLN:HE21	1.33	0.75
1:A:180:ASN:HA	1:A:185:LYS:HD2	1.67	0.75
1:F:120:LYS:HE2	1:F:120:LYS:H	1.52	0.74
1:D:275:THR:HG22	1:D:277:CYS:N	1.99	0.74
1:G:156:THR:CG2	1:G:159:GLY:H	1.99	0.74
1:E:209:MET:HB2	1:G:353:PRO:HB2	1.68	0.74
1:A:277:CYS:HB3	1:B:416:LEU:HD21	1.70	0.74
1:B:196:GLU:HG2	1:D:203:LYS:NZ	2.02	0.74
1:F:180:ASN:HA	1:F:185:LYS:HD2	1.69	0.74
1:H:180:ASN:HA	1:H:185:LYS:HD2	1.70	0.74
1:A:7:LYS:HE3	1:A:99:PHE:HB3	1.68	0.73
1:A:419:PRO:HG2	1:A:422:GLY:HA3	1.71	0.73
1:B:7:LYS:NZ	1:B:101:TRP:HE3	1.86	0.73
1:F:7:LYS:HE3	1:F:99:PHE:HB3	1.71	0.73
1:G:416:LEU:HD21	1:H:277:CYS:HB3	1.70	0.73
1:B:7:LYS:NZ	1:B:101:TRP:CE3	2.56	0.73
1:C:7:LYS:HE2	1:C:112:CYS:SG	2.28	0.73
1:E:419:PRO:HG2	1:E:422:GLY:HA3	1.70	0.73
1:C:180:ASN:HA	1:C:185:LYS:HD2	1.71	0.72
1:B:120:LYS:H	1:B:120:LYS:HE2	1.55	0.72
1:B:7:LYS:HE3	1:B:99:PHE:HB3	1.71	0.72
1:F:419:PRO:HG2	1:F:422:GLY:HA3	1.72	0.72
1:A:7:LYS:HE2	1:A:112:CYS:SG	2.30	0.72
1:A:275:THR:HG22	1:A:277:CYS:N	2.01	0.72
1:D:419:PRO:HG2	1:D:422:GLY:HA3	1.71	0.72
1:F:275:THR:HG22	1:F:277:CYS:N	1.99	0.71
1:F:203:LYS:HZ1	1:H:196:GLU:HG2	1.56	0.71
1:A:120:LYS:HE2	1:A:120:LYS:H	1.55	0.71
1:C:120:LYS:HE2	1:C:120:LYS:H	1.54	0.71
1:D:7:LYS:HE3	1:D:99:PHE:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:120:LYS:HE2	1:H:120:LYS:H	1.51	0.71
1:E:196:GLU:HG2	1:G:203:LYS:NZ	2.06	0.71
1:A:7:LYS:HZ1	1:A:100:ALA:N	1.89	0.71
1:B:105:THR:N	1:B:108:GLU:HG3	2.00	0.71
1:A:243:ILE:HG21	1:B:408:LEU:HD13	1.73	0.71
1:C:416:LEU:HD21	1:D:277:CYS:HB3	1.73	0.71
1:F:203:LYS:NZ	1:H:196:GLU:HG2	2.05	0.70
1:B:3:LYS:HE2	1:B:115:GLN:HE22	1.57	0.70
1:G:277:CYS:HB3	1:H:416:LEU:HD21	1.72	0.70
1:C:277:CYS:HB3	1:D:416:LEU:HD21	1.74	0.70
1:A:209:MET:HB2	1:C:353:PRO:HB2	1.74	0.70
1:F:7:LYS:HE2	1:F:112:CYS:SG	2.32	0.70
1:G:7:LYS:HE3	1:G:99:PHE:HB3	1.74	0.69
1:C:7:LYS:HE3	1:C:99:PHE:HB3	1.73	0.69
1:E:7:LYS:NZ	1:E:101:TRP:HE3	1.90	0.69
1:G:243:ILE:HG21	1:H:408:LEU:HD13	1.74	0.69
1:D:7:LYS:HE2	1:D:112:CYS:SG	2.33	0.69
1:B:419:PRO:HG2	1:B:422:GLY:HA3	1.74	0.69
1:H:7:LYS:NZ	1:H:101:TRP:CE3	2.60	0.69
1:G:7:LYS:HZ1	1:G:100:ALA:N	1.91	0.69
1:C:243:ILE:HG21	1:D:408:LEU:HD13	1.75	0.69
1:B:401:LEU:HD22	1:D:212:GLY:O	1.93	0.69
1:E:7:LYS:HE2	1:E:112:CYS:SG	2.33	0.69
1:A:7:LYS:NZ	1:A:101:TRP:CE3	2.60	0.69
1:A:421:ASN:HB2	4:H:440:HOH:O	1.91	0.69
1:B:353:PRO:HB2	1:D:209:MET:HB2	1.74	0.68
1:E:7:LYS:NZ	1:E:101:TRP:CE3	2.61	0.68
1:H:7:LYS:NZ	1:H:101:TRP:HE3	1.90	0.68
1:D:105:THR:N	1:D:108:GLU:HG3	2.01	0.68
1:G:74:ARG:HE	1:G:120:LYS:NZ	1.93	0.67
1:B:142:HIS:HB3	1:B:145:LEU:HD12	1.74	0.67
1:C:7:LYS:HZ1	1:C:100:ALA:N	1.93	0.67
1:D:74:ARG:HE	1:D:120:LYS:NZ	1.92	0.67
1:H:142:HIS:HB3	1:H:145:LEU:HD12	1.76	0.67
1:A:74:ARG:HE	1:A:120:LYS:NZ	1.93	0.67
1:D:7:LYS:NZ	1:D:101:TRP:CE3	2.61	0.67
1:A:196:GLU:HG2	1:C:203:LYS:HZ1	1.57	0.67
1:E:401:LEU:HD22	1:G:212:GLY:O	1.95	0.67
1:G:419:PRO:HG2	1:G:422:GLY:HA3	1.75	0.67
1:C:7:LYS:NZ	1:C:101:TRP:HE3	1.90	0.67
1:B:203:LYS:NZ	1:D:196:GLU:HG2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HZ1	1:B:100:ALA:N	1.92	0.67
1:C:7:LYS:NZ	1:C:101:TRP:CE3	2.60	0.67
1:D:421:ASN:HB3	4:D:443:HOH:O	1.96	0.66
1:G:308:LYS:H	1:G:308:LYS:CD	2.07	0.66
1:G:7:LYS:HE2	1:G:112:CYS:SG	2.34	0.66
1:D:142:HIS:HB3	1:D:145:LEU:HD12	1.76	0.66
1:F:7:LYS:HZ1	1:F:100:ALA:N	1.93	0.66
1:E:203:LYS:HZ1	1:G:196:GLU:HG2	1.60	0.66
1:E:203:LYS:NZ	1:G:196:GLU:HG2	2.11	0.66
1:H:129:ASP:OD2	1:H:135:THR:HG23	1.97	0.65
1:H:419:PRO:HG2	1:H:422:GLY:HA3	1.78	0.65
1:F:74:ARG:HE	1:F:120:LYS:NZ	1.94	0.65
1:D:7:LYS:HZ1	1:D:100:ALA:N	1.95	0.65
1:E:74:ARG:HE	1:E:120:LYS:NZ	1.94	0.65
1:E:416:LEU:HD21	1:F:277:CYS:HB3	1.78	0.65
1:F:13:LEU:HB3	1:F:86:HIS:HA	1.79	0.65
1:F:129:ASP:OD2	1:F:135:THR:HG23	1.97	0.65
1:G:7:LYS:NZ	1:G:101:TRP:CE3	2.61	0.65
1:C:142:HIS:HB3	1:C:145:LEU:HD12	1.79	0.65
1:D:13:LEU:HB3	1:D:86:HIS:HA	1.78	0.65
1:G:105:THR:N	1:G:108:GLU:HG3	2.02	0.65
1:G:408:LEU:HD13	1:H:243:ILE:HG21	1.78	0.65
1:B:74:ARG:HG3	1:B:119:PHE:CZ	2.31	0.65
1:A:13:LEU:HB3	1:A:86:HIS:HA	1.78	0.65
1:E:196:GLU:HG2	1:G:203:LYS:HZ1	1.59	0.65
1:C:13:LEU:HB3	1:C:86:HIS:HA	1.77	0.64
1:A:203:LYS:HZ1	1:C:196:GLU:HG2	1.62	0.64
1:A:275:THR:HG21	1:A:280:ILE:HD11	1.79	0.64
1:H:4:LEU:HD12	1:H:4:LEU:N	2.12	0.64
1:E:13:LEU:HB3	1:E:86:HIS:HA	1.79	0.64
1:F:196:GLU:HG2	1:H:203:LYS:NZ	2.13	0.64
1:D:4:LEU:HD11	1:D:111:TRP:CH2	2.32	0.64
1:D:74:ARG:HG3	1:D:119:PHE:CZ	2.33	0.64
1:G:7:LYS:NZ	1:G:101:TRP:HE3	1.91	0.64
1:G:74:ARG:HG3	1:G:119:PHE:CZ	2.32	0.64
1:H:278:VAL:HG12	1:H:303:VAL:HB	1.79	0.64
1:A:4:LEU:HD11	1:A:111:TRP:CH2	2.31	0.64
1:G:278:VAL:HG12	1:G:303:VAL:HB	1.80	0.64
1:B:13:LEU:HB3	1:B:86:HIS:HA	1.80	0.64
1:A:209:MET:HB2	1:C:353:PRO:CB	2.28	0.64
1:E:142:HIS:HB3	1:E:145:LEU:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ARG:HE	1:B:120:LYS:NZ	1.96	0.63
1:D:28:MET:HB3	1:D:358:SER:HB2	1.80	0.63
1:E:28:MET:HB3	1:E:358:SER:HB2	1.80	0.63
1:C:74:ARG:HE	1:C:120:LYS:NZ	1.96	0.63
1:H:7:LYS:HE2	1:H:112:CYS:SG	2.39	0.63
1:A:7:LYS:NZ	1:A:101:TRP:HE3	1.88	0.63
1:B:275:THR:HG21	1:B:280:ILE:HD11	1.78	0.63
1:F:7:LYS:NZ	1:F:101:TRP:CE3	2.61	0.63
1:H:74:ARG:HG3	1:H:119:PHE:CZ	2.33	0.63
1:E:117:LEU:HD22	1:E:138:ILE:HD11	1.81	0.63
1:B:278:VAL:HG12	1:B:303:VAL:HB	1.81	0.63
1:E:4:LEU:HD12	1:E:4:LEU:N	2.13	0.63
1:C:308:LYS:CD	1:C:308:LYS:H	2.09	0.63
1:D:300:HIS:N	2:D:432:NAD:H1D	2.12	0.63
1:F:74:ARG:HG3	1:F:119:PHE:CZ	2.33	0.63
1:E:353:PRO:HB2	1:G:209:MET:HB2	1.80	0.62
1:F:7:LYS:NZ	1:F:101:TRP:HE3	1.90	0.62
1:H:28:MET:HB3	1:H:358:SER:HB2	1.81	0.62
1:E:74:ARG:HG3	1:E:119:PHE:CZ	2.34	0.62
1:G:120:LYS:CE	1:G:120:LYS:H	2.13	0.62
1:H:13:LEU:HB3	1:H:86:HIS:HA	1.81	0.62
1:C:4:LEU:HD11	1:C:111:TRP:CH2	2.34	0.62
1:E:105:THR:N	1:E:108:GLU:HG3	2.06	0.62
1:G:275:THR:HG22	1:G:276:GLY:N	2.14	0.62
1:D:120:LYS:H	1:D:120:LYS:CE	2.12	0.62
1:D:4:LEU:N	1:D:4:LEU:HD12	2.15	0.62
1:E:129:ASP:OD2	1:E:135:THR:HG23	1.99	0.62
1:C:408:LEU:HD13	1:D:243:ILE:HG21	1.82	0.62
1:C:419:PRO:HB2	1:C:422:GLY:H	1.65	0.62
1:D:7:LYS:NZ	1:D:100:ALA:N	2.48	0.62
1:F:278:VAL:HG12	1:F:303:VAL:HB	1.82	0.62
1:G:7:LYS:NZ	1:G:100:ALA:N	2.48	0.62
1:G:129:ASP:OD2	1:G:135:THR:HG23	1.99	0.62
1:E:120:LYS:H	1:E:120:LYS:CE	2.13	0.62
1:E:7:LYS:NZ	1:E:100:ALA:N	2.47	0.62
1:A:203:LYS:NZ	1:C:196:GLU:HG2	2.15	0.62
1:G:13:LEU:HB3	1:G:86:HIS:HA	1.80	0.62
1:B:4:LEU:HD12	1:B:4:LEU:N	2.14	0.62
1:A:278:VAL:HG12	1:A:303:VAL:HB	1.82	0.61
1:A:74:ARG:HG3	1:A:119:PHE:CZ	2.34	0.61
1:E:275:THR:HG21	1:E:280:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:GLY:O	1:H:401:LEU:HD22	2.01	0.61
1:A:117:LEU:HD22	1:A:138:ILE:HD11	1.83	0.61
1:A:415:TYR:OH	1:B:303:VAL:HG21	2.00	0.61
1:A:421:ASN:ND2	1:H:312:GLU:OE2	2.33	0.61
1:B:4:LEU:HD11	1:B:111:TRP:CH2	2.36	0.61
1:C:7:LYS:NZ	1:C:100:ALA:N	2.48	0.61
1:E:3:LYS:HE2	1:E:115:GLN:HE22	1.65	0.61
1:G:117:LEU:HD22	1:G:138:ILE:HD11	1.82	0.61
1:H:7:LYS:NZ	1:H:100:ALA:N	2.49	0.61
1:A:142:HIS:HB3	1:A:145:LEU:HD12	1.82	0.61
1:C:4:LEU:HD12	1:C:4:LEU:N	2.15	0.61
1:F:105:THR:N	1:F:108:GLU:HG3	2.04	0.61
1:F:120:LYS:CE	1:F:120:LYS:H	2.13	0.61
1:B:250:GLN:O	1:B:254:GLU:HG2	2.00	0.61
1:G:4:LEU:HD12	1:G:4:LEU:N	2.14	0.61
1:H:275:THR:HG21	1:H:280:ILE:HD11	1.81	0.61
1:B:188:PHE:HA	1:B:192:TYR:CD2	2.36	0.61
1:A:353:PRO:HB2	1:C:209:MET:HB2	1.81	0.61
1:G:142:HIS:HB3	1:G:145:LEU:HD12	1.83	0.61
1:A:4:LEU:N	1:A:4:LEU:HD12	2.16	0.61
1:C:74:ARG:HG3	1:C:119:PHE:CZ	2.35	0.61
1:H:386:PRO:HG2	1:H:389:LEU:HG	1.81	0.61
1:H:7:LYS:HZ1	1:H:100:ALA:N	1.99	0.61
1:B:7:LYS:NZ	1:B:100:ALA:N	2.49	0.60
1:B:300:HIS:N	2:B:432:NAD:H1D	2.14	0.60
1:C:105:THR:N	1:C:108:GLU:HG3	2.04	0.60
1:A:7:LYS:NZ	1:A:100:ALA:N	2.49	0.60
1:B:395:GLU:HA	1:B:398:LEU:HD22	1.83	0.60
1:C:28:MET:HB3	1:C:358:SER:HB2	1.83	0.60
1:E:7:LYS:HZ1	1:E:100:ALA:N	1.99	0.60
1:F:7:LYS:NZ	1:F:100:ALA:N	2.49	0.60
1:G:7:LYS:HD3	1:G:111:TRP:CZ3	2.36	0.60
1:A:105:THR:N	1:A:108:GLU:HG3	2.05	0.60
1:B:196:GLU:HG2	1:D:203:LYS:HZ1	1.65	0.60
1:D:275:THR:HG22	1:D:276:GLY:N	2.16	0.60
1:H:74:ARG:HE	1:H:120:LYS:NZ	1.99	0.60
1:E:278:VAL:HG12	1:E:303:VAL:HB	1.83	0.60
1:C:386:PRO:HG2	1:C:389:LEU:HG	1.84	0.60
1:E:408:LEU:HD13	1:F:243:ILE:HG21	1.82	0.60
1:H:120:LYS:CE	1:H:120:LYS:H	2.15	0.60
1:C:278:VAL:HG12	1:C:303:VAL:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:LEU:HD11	1:D:111:TRP:CZ2	2.37	0.60
1:F:275:THR:HG21	1:F:280:ILE:HD11	1.83	0.60
1:F:4:LEU:N	1:F:4:LEU:HD12	2.15	0.60
1:F:188:PHE:HA	1:F:192:TYR:CD2	2.37	0.60
1:G:4:LEU:HD11	1:G:111:TRP:CH2	2.36	0.60
1:B:150:ARG:HD2	1:B:372:TRP:HA	1.84	0.60
1:B:386:PRO:HG2	1:B:389:LEU:HG	1.84	0.60
1:C:129:ASP:OD2	1:C:135:THR:HG23	2.01	0.60
1:C:150:ARG:HD2	1:C:372:TRP:HA	1.84	0.60
1:C:275:THR:HG21	1:C:280:ILE:HD11	1.83	0.60
1:D:278:VAL:HG12	1:D:303:VAL:HB	1.83	0.60
1:B:56:THR:HA	1:B:84:GLN:HB2	1.84	0.59
1:A:300:HIS:N	2:A:432:NAD:H1D	2.12	0.59
1:B:386:PRO:HD2	1:B:389:LEU:HD12	1.83	0.59
1:A:212:GLY:O	1:C:401:LEU:HD22	2.03	0.59
1:F:4:LEU:HD11	1:F:111:TRP:CH2	2.37	0.59
1:C:188:PHE:HA	1:C:192:TYR:CD2	2.37	0.59
1:E:419:PRO:HB2	1:E:422:GLY:H	1.67	0.59
1:F:117:LEU:HD22	1:F:138:ILE:HD11	1.85	0.59
1:F:300:HIS:HA	1:F:343:LEU:HD11	1.83	0.59
1:B:209:MET:HB2	1:D:353:PRO:HB2	1.85	0.59
1:D:7:LYS:NZ	1:D:101:TRP:HE3	1.89	0.59
1:D:129:ASP:OD2	1:D:135:THR:HG23	2.02	0.59
1:D:386:PRO:HG2	1:D:389:LEU:HG	1.85	0.59
1:F:209:MET:HB2	1:H:353:PRO:HB2	1.85	0.59
1:H:419:PRO:HB2	1:H:422:GLY:H	1.67	0.59
1:D:300:HIS:HA	1:D:343:LEU:HD11	1.85	0.59
1:G:188:PHE:HA	1:G:192:TYR:CD2	2.37	0.59
1:H:7:LYS:HD3	1:H:111:TRP:CZ3	2.37	0.59
1:G:150:ARG:HD2	1:G:372:TRP:HA	1.85	0.59
1:H:4:LEU:HD11	1:H:111:TRP:CH2	2.38	0.58
1:E:188:PHE:HA	1:E:192:TYR:CD2	2.38	0.58
1:F:7:LYS:CD	1:F:111:TRP:HZ3	2.17	0.58
1:B:308:LYS:CD	1:B:308:LYS:H	2.08	0.58
1:D:308:LYS:CD	1:D:308:LYS:H	2.09	0.58
1:E:275:THR:HG22	1:E:276:GLY:N	2.18	0.58
1:G:7:LYS:CD	1:G:111:TRP:HZ3	2.15	0.58
1:H:117:LEU:HD22	1:H:138:ILE:HD11	1.85	0.58
1:H:150:ARG:HD2	1:H:372:TRP:HA	1.84	0.58
1:A:419:PRO:HB2	1:A:422:GLY:H	1.68	0.58
1:C:120:LYS:H	1:C:120:LYS:CE	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:LEU:O	1:F:253:MET:HG2	2.02	0.58
1:G:7:LYS:HD3	1:G:111:TRP:HZ3	1.68	0.58
1:C:56:THR:HA	1:C:84:GLN:HB2	1.85	0.58
1:G:387:LYS:HE3	1:G:431:TYR:OH	2.03	0.58
1:A:416:LEU:CD2	1:B:277:CYS:HB3	2.33	0.58
1:G:275:THR:HG21	1:G:280:ILE:HD11	1.84	0.58
1:A:129:ASP:OD2	1:A:135:THR:HG23	2.03	0.58
1:B:188:PHE:HA	1:B:192:TYR:HD2	1.69	0.58
1:H:300:HIS:N	2:H:432:NAD:H1D	2.13	0.58
1:C:4:LEU:HD11	1:C:111:TRP:CZ2	2.39	0.58
1:A:150:ARG:HD2	1:A:372:TRP:HA	1.86	0.58
1:B:4:LEU:HD11	1:B:111:TRP:CZ2	2.39	0.58
1:B:129:ASP:OD2	1:B:135:THR:HG23	2.03	0.58
1:D:188:PHE:HA	1:D:192:TYR:CD2	2.39	0.58
1:A:386:PRO:HD2	1:A:389:LEU:HD12	1.86	0.57
1:A:56:THR:HA	1:A:84:GLN:HB2	1.86	0.57
1:A:4:LEU:HD11	1:A:111:TRP:CZ2	2.39	0.57
1:B:244:ASP:CG	1:B:247:ASN:HD22	2.07	0.57
1:F:7:LYS:HD3	1:F:111:TRP:CZ3	2.37	0.57
1:G:249:LEU:O	1:G:253:MET:HG2	2.03	0.57
1:H:105:THR:N	1:H:108:GLU:HG3	2.08	0.57
1:H:3:LYS:HE2	1:H:115:GLN:HE22	1.68	0.57
1:H:188:PHE:HA	1:H:192:TYR:CD2	2.39	0.57
1:H:7:LYS:CD	1:H:111:TRP:HZ3	2.17	0.57
1:E:308:LYS:HD2	1:E:308:LYS:N	2.15	0.57
1:G:3:LYS:HE2	1:G:115:GLN:HE22	1.68	0.57
1:B:300:HIS:HA	1:B:343:LEU:HD11	1.86	0.57
1:F:343:LEU:HG	2:F:432:NAD:N7N	2.19	0.57
1:A:300:HIS:HA	1:A:343:LEU:HD11	1.87	0.57
1:B:81:PHE:CD2	1:B:342:ARG:HD2	2.40	0.57
1:D:56:THR:HA	1:D:84:GLN:HB2	1.87	0.57
1:E:199:ILE:HG22	1:E:203:LYS:HG3	1.85	0.57
1:E:389:LEU:O	1:E:393:VAL:HG23	2.04	0.57
1:A:401:LEU:HD22	1:C:212:GLY:O	2.05	0.57
1:A:343:LEU:HG	2:A:432:NAD:N7N	2.20	0.57
1:C:117:LEU:HD22	1:C:138:ILE:HD11	1.87	0.57
1:A:209:MET:HG3	1:C:196:GLU:OE1	2.04	0.57
1:E:209:MET:HB2	1:G:353:PRO:CB	2.35	0.57
1:H:7:LYS:HE3	1:H:99:PHE:CB	2.33	0.57
1:B:3:LYS:HE2	1:B:115:GLN:NE2	2.19	0.57
1:B:117:LEU:HD22	1:B:138:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:HIS:HB2	4:B:459:HOH:O	2.05	0.57
1:D:275:THR:HG21	1:D:280:ILE:HD11	1.84	0.57
1:H:389:LEU:O	1:H:393:VAL:HG23	2.03	0.57
1:A:199:ILE:HG22	1:A:203:LYS:HG3	1.87	0.57
1:A:395:GLU:HA	1:A:398:LEU:HD22	1.86	0.57
1:B:120:LYS:CE	1:B:120:LYS:H	2.17	0.57
1:B:389:LEU:O	1:B:393:VAL:HG23	2.05	0.57
1:F:275:THR:HG22	1:F:276:GLY:N	2.19	0.57
1:E:244:ASP:CG	1:E:247:ASN:HD22	2.08	0.57
1:F:188:PHE:HA	1:F:192:TYR:HD2	1.70	0.57
1:D:249:LEU:O	1:D:253:MET:HG2	2.05	0.56
1:F:199:ILE:HG22	1:F:203:LYS:HG3	1.87	0.56
1:F:387:LYS:O	1:F:391:GLU:HG3	2.04	0.56
1:A:386:PRO:HG2	1:A:389:LEU:HG	1.88	0.56
1:C:343:LEU:HG	2:C:432:NAD:N7N	2.20	0.56
1:D:343:LEU:HG	2:D:432:NAD:N7N	2.20	0.56
1:H:4:LEU:HD12	1:H:4:LEU:H	1.70	0.56
1:H:56:THR:HA	1:H:84:GLN:HB2	1.87	0.56
1:F:250:GLN:O	1:F:254:GLU:HG2	2.06	0.56
1:A:120:LYS:H	1:A:120:LYS:CE	2.18	0.56
1:A:28:MET:HB3	1:A:358:SER:HB2	1.88	0.56
1:A:7:LYS:HE3	1:A:99:PHE:CB	2.36	0.56
1:B:387:LYS:HE3	1:B:431:TYR:OH	2.06	0.56
1:D:117:LEU:HD22	1:D:138:ILE:HD11	1.87	0.56
1:E:386:PRO:HG2	1:E:389:LEU:HG	1.87	0.56
1:F:150:ARG:HD2	1:F:372:TRP:HA	1.86	0.56
1:F:387:LYS:HE3	1:F:431:TYR:OH	2.06	0.56
1:F:389:LEU:O	1:F:393:VAL:HG23	2.06	0.56
1:H:300:HIS:HA	1:H:343:LEU:HD11	1.87	0.56
1:C:3:LYS:HE2	1:C:115:GLN:HE22	1.70	0.56
1:G:343:LEU:HG	2:G:432:NAD:N7N	2.19	0.56
1:A:3:LYS:HE2	1:A:115:GLN:HE22	1.71	0.56
1:A:407:LYS:HE2	1:A:420:ILE:HG22	1.87	0.56
1:C:300:HIS:N	2:C:432:NAD:H1D	2.14	0.56
1:E:4:LEU:HD11	1:E:111:TRP:CH2	2.39	0.56
1:E:4:LEU:HD11	1:E:111:TRP:CZ2	2.41	0.56
1:G:300:HIS:HA	1:G:343:LEU:HD11	1.86	0.56
1:G:430:ARG:HB3	1:H:430:ARG:HB3	1.87	0.56
1:E:300:HIS:N	2:E:432:NAD:H1D	2.14	0.56
1:F:142:HIS:HB3	1:F:145:LEU:HD12	1.86	0.56
1:A:188:PHE:HA	1:A:192:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ASN:O	1:D:166:MET:HG3	2.06	0.56
1:F:419:PRO:HB2	1:F:422:GLY:H	1.71	0.56
1:F:300:HIS:N	2:F:432:NAD:H1D	2.13	0.56
1:G:386:PRO:HG2	1:G:389:LEU:HG	1.87	0.56
1:A:389:LEU:O	1:A:393:VAL:HG23	2.06	0.56
1:D:150:ARG:HD2	1:D:372:TRP:HA	1.87	0.56
1:E:308:LYS:CD	1:E:308:LYS:H	2.05	0.56
1:E:395:GLU:HA	1:E:398:LEU:HD22	1.86	0.56
1:H:387:LYS:HE3	1:H:431:TYR:OH	2.05	0.56
1:B:199:ILE:HG22	1:B:203:LYS:HG3	1.87	0.56
1:F:28:MET:HB3	1:F:358:SER:HB2	1.88	0.56
1:G:4:LEU:HD11	1:G:111:TRP:CZ2	2.41	0.56
1:H:4:LEU:HD11	1:H:111:TRP:CZ2	2.41	0.56
1:A:138:ILE:HG22	1:A:146:LEU:HD13	1.88	0.56
1:C:185:LYS:C	1:C:185:LYS:HD3	2.26	0.56
1:F:141:LYS:HB3	1:F:142:HIS:ND1	2.21	0.56
1:F:3:LYS:HE2	1:F:115:GLN:HE22	1.70	0.56
1:E:141:LYS:HB3	1:E:142:HIS:ND1	2.21	0.55
1:G:300:HIS:N	2:G:432:NAD:H1D	2.14	0.55
1:B:7:LYS:CD	1:B:111:TRP:HZ3	2.20	0.55
1:G:199:ILE:HG22	1:G:203:LYS:HG3	1.87	0.55
1:D:387:LYS:O	1:D:391:GLU:HG3	2.06	0.55
1:E:343:LEU:HG	2:E:432:NAD:N7N	2.21	0.55
1:A:308:LYS:HD2	1:A:308:LYS:N	2.15	0.55
1:E:430:ARG:HB3	1:F:430:ARG:HB3	1.88	0.55
1:G:107:GLU:HG2	4:G:451:HOH:O	2.06	0.55
1:H:199:ILE:HG22	1:H:203:LYS:HG3	1.87	0.55
1:A:275:THR:HG22	1:A:276:GLY:N	2.21	0.55
1:B:7:LYS:HD3	1:B:111:TRP:CZ3	2.41	0.55
1:B:24:ALA:O	1:B:28:MET:HG3	2.06	0.55
1:C:275:THR:HG22	1:C:276:GLY:N	2.21	0.55
1:C:407:LYS:HE2	1:C:420:ILE:HG22	1.88	0.55
1:D:143:PRO:O	1:D:146:LEU:HB2	2.06	0.55
1:H:343:LEU:HG	2:H:432:NAD:N7N	2.21	0.55
1:C:162:ASN:HB2	4:C:460:HOH:O	2.05	0.55
1:D:250:GLN:O	1:D:254:GLU:HG2	2.07	0.55
1:F:308:LYS:H	1:F:308:LYS:CD	2.09	0.55
1:E:7:LYS:HE3	1:E:99:PHE:CB	2.34	0.55
1:F:386:PRO:HD2	1:F:389:LEU:HD12	1.88	0.55
1:C:389:LEU:O	1:C:393:VAL:HG23	2.07	0.55
1:C:430:ARG:HB3	1:D:430:ARG:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:THR:HA	1:F:84:GLN:HB2	1.87	0.55
1:G:386:PRO:HD2	1:G:389:LEU:HD12	1.88	0.55
1:B:162:ASN:O	1:B:166:MET:HG3	2.07	0.55
1:C:143:PRO:O	1:C:146:LEU:HB2	2.07	0.55
1:F:185:LYS:C	1:F:185:LYS:HD3	2.27	0.55
1:F:4:LEU:HD11	1:F:111:TRP:CZ2	2.41	0.55
1:H:185:LYS:HD3	1:H:185:LYS:C	2.27	0.55
1:G:308:LYS:N	1:G:308:LYS:HD2	2.17	0.54
1:G:56:THR:HA	1:G:84:GLN:HB2	1.88	0.54
1:C:387:LYS:HE3	1:C:431:TYR:OH	2.08	0.54
1:B:212:GLY:O	1:D:401:LEU:HD22	2.06	0.54
1:D:81:PHE:CD2	1:D:342:ARG:HD2	2.43	0.54
1:E:300:HIS:HA	1:E:343:LEU:HD11	1.89	0.54
1:E:150:ARG:HD2	1:E:372:TRP:HA	1.89	0.54
1:B:353:PRO:CB	1:D:209:MET:HB2	2.36	0.54
1:C:386:PRO:HD2	1:C:389:LEU:HD12	1.89	0.54
1:E:56:THR:HA	1:E:84:GLN:HB2	1.88	0.54
1:G:131:GLY:HA2	1:G:156:THR:HG21	1.89	0.54
1:C:138:ILE:HG22	1:C:146:LEU:HD13	1.90	0.54
1:D:141:LYS:HB3	1:D:142:HIS:ND1	2.21	0.54
1:H:179:VAL:HG13	1:H:363:ASN:HB3	1.89	0.54
1:F:7:LYS:HD3	1:F:111:TRP:HZ3	1.72	0.54
1:H:308:LYS:CD	1:H:308:LYS:H	2.09	0.54
1:A:250:GLN:O	1:A:254:GLU:HG2	2.07	0.54
1:E:131:GLY:HA2	1:E:156:THR:HG21	1.90	0.54
1:F:138:ILE:HG22	1:F:146:LEU:HD13	1.89	0.54
1:H:250:GLN:O	1:H:254:GLU:HG2	2.08	0.54
1:B:141:LYS:HB3	1:B:142:HIS:ND1	2.23	0.54
1:C:395:GLU:HA	1:C:398:LEU:HD22	1.88	0.54
1:E:7:LYS:HD3	1:E:111:TRP:CZ3	2.43	0.54
1:B:249:LEU:O	1:B:253:MET:HG2	2.07	0.54
1:C:249:LEU:O	1:C:253:MET:HG2	2.08	0.54
1:G:162:ASN:O	1:G:166:MET:HG3	2.07	0.54
1:G:395:GLU:HA	1:G:398:LEU:HD22	1.88	0.54
1:B:343:LEU:HG	2:B:432:NAD:N7N	2.22	0.54
1:D:386:PRO:HD2	1:D:389:LEU:HD12	1.89	0.54
1:E:24:ALA:O	1:E:28:MET:HG3	2.08	0.54
1:H:138:ILE:HG22	1:H:146:LEU:HD13	1.89	0.54
1:B:142:HIS:CB	1:B:145:LEU:HD12	2.38	0.53
1:B:419:PRO:HB2	1:B:422:GLY:H	1.74	0.53
1:D:4:LEU:H	1:D:4:LEU:HD12	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:LYS:O	1:E:45:LYS:HG3	2.07	0.53
1:E:4:LEU:HD12	1:E:4:LEU:H	1.72	0.53
1:F:74:ARG:HG3	1:F:119:PHE:CE2	2.43	0.53
1:H:7:LYS:HD3	1:H:111:TRP:HZ3	1.71	0.53
1:D:142:HIS:CB	1:D:145:LEU:HD12	2.37	0.53
1:H:275:THR:HG22	1:H:276:GLY:N	2.22	0.53
1:A:81:PHE:CD2	1:A:342:ARG:HD2	2.43	0.53
1:C:7:LYS:HD3	1:C:111:TRP:CZ3	2.44	0.53
1:B:203:LYS:HZ1	1:D:196:GLU:HG2	1.71	0.53
1:D:244:ASP:CG	1:D:247:ASN:HD22	2.12	0.53
1:H:308:LYS:HD2	1:H:308:LYS:N	2.20	0.53
1:D:183:VAL:HG21	1:D:431:TYR:CE1	2.43	0.53
1:D:419:PRO:HB2	1:D:422:GLY:H	1.73	0.53
1:D:3:LYS:HE2	1:D:115:GLN:HE22	1.73	0.53
1:F:162:ASN:O	1:F:166:MET:HG3	2.09	0.53
1:B:275:THR:HG22	1:B:276:GLY:N	2.24	0.53
1:D:183:VAL:HA	4:D:434:HOH:O	2.08	0.53
1:E:249:LEU:O	1:E:253:MET:HG2	2.09	0.53
1:E:386:PRO:HD2	1:E:389:LEU:HD12	1.91	0.53
1:E:407:LYS:HE3	4:E:468:HOH:O	2.09	0.53
1:E:7:LYS:CD	1:E:111:TRP:HZ3	2.21	0.53
1:G:389:LEU:O	1:G:393:VAL:HG23	2.08	0.53
1:A:141:LYS:HB3	1:A:142:HIS:ND1	2.23	0.53
1:D:161:HIS:CD2	1:D:165:LYS:HZ1	2.26	0.53
1:H:183:VAL:HG21	1:H:431:TYR:CE1	2.44	0.53
1:A:162:ASN:O	1:A:166:MET:HG3	2.08	0.53
1:B:4:LEU:HD12	1:B:4:LEU:H	1.73	0.53
1:B:7:LYS:HE3	1:B:99:PHE:CB	2.38	0.53
1:C:183:VAL:HG21	1:C:431:TYR:CE1	2.44	0.53
1:C:308:LYS:N	1:C:308:LYS:HD2	2.18	0.53
1:F:386:PRO:HG2	1:F:389:LEU:HG	1.90	0.53
1:F:407:LYS:HE2	1:F:420:ILE:HG22	1.89	0.53
1:H:141:LYS:HB3	1:H:142:HIS:ND1	2.24	0.53
1:A:24:ALA:O	1:A:28:MET:HG3	2.09	0.53
1:C:81:PHE:CD2	1:C:342:ARG:HD2	2.43	0.53
1:D:199:ILE:HG22	1:D:203:LYS:HG3	1.89	0.53
1:D:387:LYS:HE3	1:D:431:TYR:OH	2.09	0.53
1:D:389:LEU:O	1:D:393:VAL:HG23	2.08	0.53
1:G:74:ARG:HG3	1:G:119:PHE:CE2	2.44	0.53
1:C:300:HIS:HA	1:C:343:LEU:HD11	1.91	0.52
1:D:366:MET:HG3	4:D:467:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ASN:O	1:E:166:MET:HG3	2.09	0.52
1:G:188:PHE:HA	1:G:192:TYR:HD2	1.73	0.52
1:G:4:LEU:HD12	1:G:4:LEU:H	1.74	0.52
1:A:185:LYS:HD3	1:A:185:LYS:C	2.29	0.52
1:B:143:PRO:O	1:B:146:LEU:HB2	2.09	0.52
1:C:152:ILE:HG22	1:C:153:SER:N	2.24	0.52
1:C:181:ASP:HB2	1:C:384:PHE:HE1	1.73	0.52
1:D:7:LYS:HE3	1:D:99:PHE:CB	2.38	0.52
1:E:161:HIS:CD2	1:E:161:HIS:C	2.83	0.52
1:H:143:PRO:O	1:H:146:LEU:HB2	2.10	0.52
1:B:194:CYS:SG	1:B:223:VAL:HG13	2.50	0.52
1:D:7:LYS:CD	1:D:111:TRP:HZ3	2.22	0.52
1:F:353:PRO:CB	1:H:209:MET:HB2	2.37	0.52
1:B:74:ARG:HG3	1:B:119:PHE:CE2	2.43	0.52
1:B:7:LYS:CE	1:B:101:TRP:HZ3	2.23	0.52
1:B:7:LYS:HZ1	1:B:100:ALA:CA	2.23	0.52
1:C:4:LEU:HD12	1:C:4:LEU:H	1.74	0.52
1:E:407:LYS:HE2	1:E:420:ILE:HG22	1.92	0.52
1:G:110:LEU:O	1:G:110:LEU:HD22	2.10	0.52
1:G:143:PRO:O	1:G:146:LEU:HB2	2.09	0.52
1:G:81:PHE:CD2	1:G:342:ARG:HD2	2.44	0.52
1:H:244:ASP:CG	1:H:247:ASN:HD22	2.12	0.52
1:B:361:PHE:O	1:B:365:VAL:HG23	2.09	0.52
1:D:74:ARG:HG2	4:D:444:HOH:O	2.08	0.52
1:E:243:ILE:HG21	1:F:408:LEU:CD1	2.38	0.52
1:E:343:LEU:HD23	1:E:346:LEU:HD12	1.92	0.52
1:A:4:LEU:H	1:A:4:LEU:HD12	1.75	0.52
1:B:105:THR:OG1	1:B:108:GLU:HG2	2.10	0.52
1:C:74:ARG:HE	1:C:120:LYS:HZ1	1.58	0.52
1:E:31:LEU:HD13	1:E:61:VAL:HG12	1.92	0.52
1:F:81:PHE:CD2	1:F:342:ARG:HD2	2.44	0.52
1:H:386:PRO:HD2	1:H:389:LEU:HD12	1.90	0.52
1:H:48:ARG:HD2	1:H:119:PHE:HB2	1.92	0.52
1:C:7:LYS:HZ1	1:C:100:ALA:CA	2.22	0.52
1:E:387:LYS:O	1:E:391:GLU:HG3	2.09	0.52
1:E:138:ILE:HG22	1:E:146:LEU:HD13	1.92	0.52
1:F:24:ALA:O	1:F:28:MET:HG3	2.10	0.52
1:A:74:ARG:HG3	1:A:119:PHE:CE2	2.45	0.52
1:A:387:LYS:HE3	1:A:431:TYR:OH	2.10	0.52
1:B:7:LYS:HD3	1:B:111:TRP:HZ3	1.75	0.52
1:C:244:ASP:CG	1:C:247:ASN:HD22	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LYS:HD3	1:D:111:TRP:CZ3	2.45	0.52
1:E:143:PRO:O	1:E:146:LEU:HB2	2.08	0.52
1:E:387:LYS:HE3	1:E:431:TYR:OH	2.09	0.52
1:G:161:HIS:CD2	1:G:161:HIS:C	2.83	0.52
1:C:48:ARG:HD2	1:C:119:PHE:CB	2.39	0.52
1:C:7:LYS:CD	1:C:111:TRP:HZ3	2.22	0.52
1:H:74:ARG:HG3	1:H:119:PHE:CE2	2.44	0.52
1:H:249:LEU:O	1:H:253:MET:HG2	2.10	0.52
1:H:81:PHE:CD2	1:H:342:ARG:HD2	2.45	0.52
1:A:179:VAL:HG13	1:A:363:ASN:HB3	1.92	0.51
1:G:361:PHE:O	1:G:365:VAL:HG23	2.09	0.51
1:H:142:HIS:CB	1:H:145:LEU:HD12	2.40	0.51
1:F:143:PRO:O	1:F:146:LEU:HB2	2.10	0.51
1:G:48:ARG:HD2	1:G:119:PHE:CB	2.40	0.51
1:E:210:ILE:N	1:G:196:GLU:OE1	2.44	0.51
1:G:343:LEU:HD23	1:G:346:LEU:HD12	1.92	0.51
1:B:93:LYS:HG3	1:B:93:LYS:O	2.10	0.51
1:C:141:LYS:HB3	1:C:142:HIS:ND1	2.25	0.51
1:C:161:HIS:CD2	1:C:161:HIS:C	2.83	0.51
1:D:161:HIS:C	1:D:161:HIS:CD2	2.83	0.51
1:D:185:LYS:C	1:D:185:LYS:HD3	2.30	0.51
1:E:179:VAL:HG13	1:E:363:ASN:HB3	1.93	0.51
1:H:387:LYS:O	1:H:391:GLU:HG3	2.10	0.51
1:B:379:PRO:O	1:B:383:HIS:HE1	1.94	0.51
1:C:142:HIS:CB	1:C:145:LEU:HD12	2.40	0.51
1:F:6:TYR:OH	1:F:11:ILE:HD13	2.10	0.51
1:A:7:LYS:HD3	1:A:111:TRP:CZ3	2.46	0.51
1:C:74:ARG:HG3	1:C:119:PHE:CE2	2.46	0.51
1:D:7:LYS:HZ1	1:D:100:ALA:CA	2.24	0.51
1:E:188:PHE:HA	1:E:192:TYR:HD2	1.76	0.51
1:F:161:HIS:CD2	1:F:161:HIS:C	2.84	0.51
1:G:93:LYS:HG3	1:G:93:LYS:O	2.11	0.51
1:B:387:LYS:O	1:B:391:GLU:HG3	2.10	0.51
1:C:48:ARG:HD2	1:C:119:PHE:HB2	1.92	0.51
1:E:91:ILE:HG23	1:E:96:ILE:HB	1.93	0.51
1:F:7:LYS:HE3	1:F:99:PHE:CB	2.38	0.51
1:C:188:PHE:HA	1:C:192:TYR:HD2	1.74	0.51
1:G:419:PRO:HB2	1:G:422:GLY:H	1.74	0.51
1:H:17:GLY:HA3	1:H:86:HIS:O	2.10	0.51
1:A:188:PHE:HA	1:A:192:TYR:HD2	1.76	0.51
1:A:387:LYS:O	1:A:391:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:TYR:HE2	1:B:277:CYS:HA	1.74	0.51
1:A:4:LEU:HD11	1:A:111:TRP:HH2	1.76	0.51
1:C:343:LEU:HD23	1:C:346:LEU:HD12	1.92	0.51
1:C:361:PHE:O	1:C:365:VAL:HG23	2.11	0.51
1:C:93:LYS:O	1:C:93:LYS:HG3	2.11	0.51
1:D:379:PRO:O	1:D:383:HIS:HE1	1.93	0.51
1:D:395:GLU:HA	1:D:398:LEU:HD22	1.92	0.51
1:C:199:ILE:HG22	1:C:203:LYS:HG3	1.93	0.51
1:F:308:LYS:HD2	1:F:308:LYS:N	2.21	0.51
1:C:131:GLY:HA2	1:C:156:THR:HG21	1.93	0.51
1:D:24:ALA:O	1:D:28:MET:HG3	2.11	0.51
1:E:152:ILE:HG22	1:E:153:SER:N	2.26	0.51
1:F:343:LEU:HD23	1:F:346:LEU:HD12	1.93	0.51
1:G:387:LYS:O	1:G:391:GLU:HG3	2.10	0.51
1:A:7:LYS:CD	1:A:111:TRP:HZ3	2.24	0.50
1:D:188:PHE:HA	1:D:192:TYR:HD2	1.75	0.50
1:D:179:VAL:HG13	1:D:363:ASN:HB3	1.93	0.50
1:G:24:ALA:O	1:G:28:MET:HG3	2.11	0.50
1:C:45:LYS:O	1:C:45:LYS:HG3	2.11	0.50
1:E:74:ARG:HG3	1:E:119:PHE:CE2	2.46	0.50
1:E:300:HIS:HB2	2:E:432:NAD:O2D	2.11	0.50
1:F:120:LYS:CD	1:F:120:LYS:H	2.23	0.50
1:F:154:GLU:HG3	1:F:160:VAL:HG23	1.93	0.50
1:F:91:ILE:HG23	1:F:96:ILE:HB	1.93	0.50
1:A:181:ASP:HB2	1:A:384:PHE:HE1	1.75	0.50
1:A:183:VAL:HG21	1:A:431:TYR:CE1	2.45	0.50
1:B:188:PHE:O	1:B:192:TYR:HB2	2.12	0.50
1:B:48:ARG:HD2	1:B:119:PHE:HB2	1.92	0.50
1:C:250:GLN:O	1:C:254:GLU:HG2	2.11	0.50
1:D:407:LYS:HE2	1:D:420:ILE:HG22	1.92	0.50
1:B:48:ARG:HD2	1:B:119:PHE:CB	2.41	0.50
1:C:162:ASN:O	1:C:166:MET:HG3	2.10	0.50
1:G:141:LYS:HB3	1:G:142:HIS:ND1	2.27	0.50
1:G:142:HIS:N	1:G:143:PRO:HD3	2.26	0.50
1:G:250:GLN:O	1:G:254:GLU:HG2	2.11	0.50
1:B:142:HIS:N	1:B:143:PRO:HD3	2.26	0.50
1:B:343:LEU:HD23	1:B:346:LEU:HD12	1.92	0.50
1:D:138:ILE:HG22	1:D:146:LEU:HD13	1.92	0.50
1:E:7:LYS:CE	1:E:101:TRP:HZ3	2.25	0.50
1:A:131:GLY:HA2	1:A:156:THR:HG21	1.93	0.50
1:B:189:ASP:OD1	1:B:189:ASP:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:HIS:N	1:C:143:PRO:HD3	2.26	0.50
1:D:6:TYR:C	1:D:6:TYR:CD1	2.84	0.50
1:E:142:HIS:CB	1:E:145:LEU:HD12	2.41	0.50
1:A:244:ASP:CG	1:A:247:ASN:HD22	2.15	0.50
1:C:7:LYS:HE3	1:C:99:PHE:CB	2.40	0.50
1:F:4:LEU:HD13	1:F:99:PHE:HE1	1.77	0.50
1:G:28:MET:HB3	1:G:358:SER:HB2	1.93	0.50
1:G:45:LYS:HG3	1:G:45:LYS:O	2.09	0.50
1:A:7:LYS:HZ1	1:A:100:ALA:CA	2.24	0.50
1:B:138:ILE:HG22	1:B:146:LEU:HD13	1.93	0.50
1:C:54:HIS:CD2	1:C:54:HIS:H	2.29	0.50
1:D:142:HIS:N	1:D:143:PRO:HD3	2.27	0.50
1:D:181:ASP:HB2	1:D:384:PHE:HE1	1.77	0.50
1:A:143:PRO:O	1:A:146:LEU:HB2	2.12	0.50
1:A:425:LYS:HE2	1:B:247:ASN:HD21	1.77	0.50
1:B:183:VAL:HG21	1:B:431:TYR:CE1	2.46	0.50
1:B:179:VAL:HG13	1:B:363:ASN:HB3	1.94	0.50
1:C:57:VAL:H	1:C:84:GLN:NE2	2.10	0.50
1:D:131:GLY:HA2	1:D:156:THR:HG21	1.93	0.50
1:E:81:PHE:CD2	1:E:342:ARG:HD2	2.46	0.50
1:G:7:LYS:HZ1	1:G:100:ALA:CA	2.25	0.50
1:H:91:ILE:HG23	1:H:96:ILE:HB	1.93	0.50
1:B:57:VAL:H	1:B:84:GLN:NE2	2.09	0.49
1:C:373:THR:HG22	1:C:374:HIS:CD2	2.46	0.49
1:D:180:ASN:O	1:D:186:SER:HB2	2.12	0.49
1:E:250:GLN:O	1:E:254:GLU:HG2	2.11	0.49
1:F:152:ILE:HG13	1:F:174:VAL:HG22	1.94	0.49
1:C:179:VAL:HG13	1:C:363:ASN:HB3	1.95	0.49
1:F:74:ARG:HE	1:F:120:LYS:HZ1	1.60	0.49
1:G:275:THR:CG2	1:G:276:GLY:N	2.75	0.49
1:G:48:ARG:HD2	1:G:119:PHE:HB2	1.93	0.49
1:G:7:LYS:HE3	1:G:99:PHE:CB	2.40	0.49
1:H:142:HIS:N	1:H:143:PRO:HD3	2.27	0.49
1:F:179:VAL:HG13	1:F:363:ASN:HB3	1.94	0.49
1:F:307:VAL:H	1:F:308:LYS:NZ	2.10	0.49
1:H:101:TRP:HZ2	1:H:108:GLU:OE1	1.95	0.49
1:H:152:ILE:HG22	1:H:153:SER:N	2.28	0.49
1:H:154:GLU:HG3	1:H:160:VAL:HG23	1.95	0.49
1:A:430:ARG:HB3	1:B:430:ARG:HB3	1.94	0.49
1:E:142:HIS:N	1:E:143:PRO:HD3	2.27	0.49
1:E:361:PHE:O	1:E:365:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:LYS:CE	1:F:101:TRP:HZ3	2.25	0.49
1:G:53:LEU:O	1:G:54:HIS:C	2.51	0.49
1:H:7:LYS:CE	1:H:101:TRP:HZ3	2.25	0.49
1:A:7:LYS:CE	1:A:101:TRP:HZ3	2.26	0.49
1:B:181:ASP:HB2	1:B:384:PHE:HE1	1.77	0.49
1:C:121:ASP:N	1:C:121:ASP:OD1	2.46	0.49
1:D:154:GLU:HG3	1:D:160:VAL:HG23	1.95	0.49
1:E:105:THR:OG1	1:E:108:GLU:HG2	2.12	0.49
1:E:419:PRO:CG	1:E:422:GLY:HA3	2.41	0.49
1:G:105:THR:OG1	1:G:108:GLU:HG2	2.11	0.49
1:G:44:LEU:HB3	1:G:71:ALA:HB2	1.95	0.49
1:G:74:ARG:HE	1:G:120:LYS:HZ1	1.60	0.49
1:H:48:ARG:HD2	1:H:119:PHE:CB	2.41	0.49
1:H:162:ASN:O	1:H:166:MET:HG3	2.11	0.49
1:H:407:LYS:HE2	1:H:420:ILE:HG22	1.95	0.49
1:H:54:HIS:CD2	1:H:54:HIS:H	2.28	0.49
1:A:196:GLU:OE1	1:C:209:MET:HG3	2.12	0.49
1:A:308:LYS:CD	1:A:308:LYS:H	2.07	0.49
1:A:415:TYR:CE2	1:B:277:CYS:HA	2.48	0.49
1:C:161:HIS:CD2	1:C:165:LYS:HZ1	2.31	0.49
1:D:142:HIS:N	1:D:143:PRO:CD	2.76	0.49
1:D:45:LYS:HG3	1:D:45:LYS:O	2.12	0.49
1:E:185:LYS:C	1:E:185:LYS:HD3	2.32	0.49
1:F:105:THR:OG1	1:F:108:GLU:HG2	2.12	0.49
1:G:7:LYS:CE	1:G:101:TRP:HZ3	2.25	0.49
1:B:91:ILE:HG23	1:B:96:ILE:HB	1.95	0.49
1:D:91:ILE:HG23	1:D:96:ILE:HB	1.95	0.49
1:E:194:CYS:SG	1:E:223:VAL:HG13	2.53	0.49
1:A:48:ARG:HD2	1:A:119:PHE:CB	2.43	0.49
1:A:154:GLU:HG3	1:A:160:VAL:HG23	1.95	0.49
1:A:7:LYS:HE3	1:A:99:PHE:CA	2.43	0.49
1:B:196:GLU:OE1	1:D:210:ILE:N	2.46	0.49
1:D:194:CYS:SG	1:D:223:VAL:HG13	2.53	0.49
1:D:343:LEU:HD23	1:D:346:LEU:HD12	1.94	0.49
1:D:419:PRO:CG	1:D:422:GLY:HA3	2.41	0.49
1:A:343:LEU:HD23	1:A:346:LEU:HD12	1.94	0.49
1:B:120:LYS:CD	1:B:120:LYS:H	2.26	0.49
1:B:185:LYS:C	1:B:185:LYS:HD3	2.33	0.49
1:B:407:LYS:HE2	1:B:420:ILE:HG22	1.94	0.49
1:B:7:LYS:HE3	1:B:99:PHE:CA	2.43	0.49
1:C:7:LYS:CE	1:C:101:TRP:HZ3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:LYS:HD3	1:E:111:TRP:HZ3	1.78	0.49
1:F:4:LEU:H	1:F:4:LEU:HD12	1.74	0.49
1:G:120:LYS:CD	1:G:120:LYS:H	2.26	0.49
1:G:138:ILE:HG22	1:G:146:LEU:HD13	1.94	0.49
1:H:188:PHE:HA	1:H:192:TYR:HD2	1.76	0.49
1:A:10:ASP:HB3	1:A:13:LEU:HD22	1.95	0.49
1:D:74:ARG:HE	1:D:120:LYS:HZ1	1.58	0.49
1:G:183:VAL:HG21	1:G:431:TYR:CE1	2.48	0.49
1:A:45:LYS:O	1:A:45:LYS:HG3	2.13	0.48
1:B:161:HIS:C	1:B:161:HIS:CD2	2.86	0.48
1:F:7:LYS:HZ1	1:F:100:ALA:CA	2.26	0.48
1:A:249:LEU:O	1:A:253:MET:HG2	2.13	0.48
1:B:154:GLU:HG3	1:B:160:VAL:HG23	1.95	0.48
1:A:415:TYR:HD2	1:B:277:CYS:HB2	1.78	0.48
1:C:379:PRO:O	1:C:383:HIS:HE1	1.96	0.48
1:A:105:THR:OG1	1:A:108:GLU:HG2	2.13	0.48
1:E:10:ASP:HB3	1:E:13:LEU:HD22	1.95	0.48
1:F:244:ASP:CG	1:F:247:ASN:HD22	2.16	0.48
1:G:152:ILE:HG22	1:G:153:SER:N	2.28	0.48
1:H:161:HIS:CD2	1:H:161:HIS:C	2.87	0.48
1:A:161:HIS:C	1:A:161:HIS:CD2	2.87	0.48
1:A:48:ARG:HD2	1:A:119:PHE:HB2	1.95	0.48
1:A:74:ARG:HE	1:A:120:LYS:HZ1	1.57	0.48
1:A:91:ILE:HG23	1:A:96:ILE:HB	1.95	0.48
1:D:275:THR:CG2	1:D:276:GLY:N	2.77	0.48
1:F:373:THR:HG22	1:F:374:HIS:CD2	2.48	0.48
1:G:54:HIS:HA	1:G:77:SER:OG	2.13	0.48
1:B:142:HIS:N	1:B:143:PRO:CD	2.77	0.48
1:D:105:THR:OG1	1:D:108:GLU:HG2	2.13	0.48
1:G:179:VAL:HG13	1:G:363:ASN:HB3	1.96	0.48
1:H:181:ASP:HB2	1:H:384:PHE:HE1	1.79	0.48
1:H:189:ASP:OD1	1:H:189:ASP:C	2.52	0.48
1:H:343:LEU:HD23	1:H:346:LEU:HD12	1.96	0.48
1:A:138:ILE:HG22	1:A:146:LEU:CD1	2.44	0.48
1:B:54:HIS:H	1:B:54:HIS:CD2	2.31	0.48
1:G:181:ASP:HB2	1:G:384:PHE:HE1	1.79	0.48
1:D:308:LYS:N	1:D:308:LYS:HD2	2.17	0.48
1:F:142:HIS:N	1:F:143:PRO:HD3	2.28	0.48
1:F:131:GLY:HA2	1:F:156:THR:HG21	1.94	0.48
1:C:154:GLU:HG3	1:C:160:VAL:HG23	1.96	0.48
1:F:197:SER:OG	1:F:352:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:GLU:HA	1:H:398:LEU:HD22	1.94	0.48
1:B:275:THR:HB	1:B:304:GLU:OE1	2.14	0.48
1:C:111:TRP:O	1:C:115:GLN:HG2	2.14	0.48
1:A:353:PRO:CB	1:C:209:MET:HB2	2.44	0.48
1:C:419:PRO:CG	1:C:422:GLY:HA3	2.40	0.48
1:D:152:ILE:HG22	1:D:153:SER:N	2.29	0.48
1:D:34:MET:HE2	4:D:467:HOH:O	2.14	0.48
1:F:183:VAL:HG21	1:F:431:TYR:CE1	2.49	0.48
1:A:142:HIS:N	1:A:143:PRO:HD3	2.28	0.48
1:C:7:LYS:CD	1:C:101:TRP:HZ3	2.27	0.48
1:E:247:ASN:HD21	1:F:425:LYS:HE2	1.78	0.48
1:F:45:LYS:HG3	1:F:45:LYS:O	2.12	0.48
1:A:142:HIS:CB	1:A:145:LEU:HD12	2.44	0.47
1:C:6:TYR:C	1:C:6:TYR:CD1	2.87	0.47
1:D:54:HIS:HA	1:D:77:SER:OG	2.14	0.47
1:G:152:ILE:HG13	1:G:174:VAL:HG22	1.95	0.47
1:G:377:LYS:HD2	1:G:378:TYR:CE1	2.49	0.47
1:H:131:GLY:HA2	1:H:156:THR:HG21	1.95	0.47
1:C:105:THR:OG1	1:C:108:GLU:HG2	2.14	0.47
1:E:154:GLU:HG3	1:E:160:VAL:HG23	1.96	0.47
1:E:93:LYS:O	1:E:93:LYS:HG3	2.14	0.47
1:C:63:ILE:HG23	1:C:73:VAL:HG21	1.96	0.47
1:D:343:LEU:HG	2:D:432:NAD:H71N	1.79	0.47
1:F:379:PRO:O	1:F:383:HIS:HE1	1.97	0.47
1:G:142:HIS:N	1:G:143:PRO:CD	2.78	0.47
1:H:379:PRO:O	1:H:383:HIS:HE1	1.97	0.47
1:H:7:LYS:HE3	1:H:99:PHE:CA	2.44	0.47
1:B:131:GLY:HA2	1:B:156:THR:HG21	1.96	0.47
1:B:152:ILE:HG22	1:B:153:SER:N	2.29	0.47
1:C:165:LYS:HE3	1:C:165:LYS:HB2	1.67	0.47
1:E:189:ASP:C	1:E:189:ASP:OD1	2.52	0.47
1:F:194:CYS:SG	1:F:223:VAL:HG13	2.55	0.47
1:F:395:GLU:HA	1:F:398:LEU:HD22	1.96	0.47
1:F:93:LYS:O	1:F:93:LYS:HG3	2.13	0.47
1:H:10:ASP:HB3	1:H:13:LEU:HD22	1.95	0.47
1:A:188:PHE:O	1:A:192:TYR:HB2	2.14	0.47
1:G:185:LYS:HD3	1:G:185:LYS:C	2.35	0.47
1:H:361:PHE:O	1:H:365:VAL:HG23	2.15	0.47
1:A:165:LYS:HE3	1:A:165:LYS:HB2	1.69	0.47
1:A:259:THR:HG23	1:B:404:LYS:HG3	1.94	0.47
1:C:120:LYS:H	1:C:120:LYS:CD	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:HIS:N	1:C:143:PRO:CD	2.77	0.47
1:C:4:LEU:HD13	1:C:99:PHE:HE1	1.79	0.47
1:D:110:LEU:O	1:D:110:LEU:HD22	2.14	0.47
1:D:121:ASP:OD1	1:D:121:ASP:N	2.45	0.47
1:E:57:VAL:H	1:E:84:GLN:NE2	2.13	0.47
1:E:7:LYS:HE3	1:E:99:PHE:CA	2.45	0.47
1:F:189:ASP:C	1:F:189:ASP:OD1	2.53	0.47
1:F:300:HIS:HB2	2:F:432:NAD:O2D	2.15	0.47
1:F:48:ARG:HD2	1:F:119:PHE:HB2	1.96	0.47
1:F:31:LEU:HD13	1:F:61:VAL:HG12	1.97	0.47
1:G:373:THR:HG22	1:G:374:HIS:CD2	2.49	0.47
1:G:63:ILE:HG23	1:G:73:VAL:HG21	1.95	0.47
1:C:24:ALA:O	1:C:28:MET:HG3	2.14	0.47
1:D:7:LYS:CE	1:D:101:TRP:HZ3	2.27	0.47
1:E:275:THR:CG2	1:E:276:GLY:N	2.77	0.47
1:G:142:HIS:CB	1:G:145:LEU:HD12	2.44	0.47
1:G:244:ASP:CG	1:G:247:ASN:HD22	2.17	0.47
1:H:424:PHE:C	1:H:425:LYS:HG2	2.35	0.47
1:B:6:TYR:CD1	1:B:6:TYR:C	2.88	0.47
1:C:35:ARG:NH2	1:C:64:GLU:HB2	2.30	0.47
1:E:48:ARG:HD2	1:E:119:PHE:CB	2.44	0.47
1:F:142:HIS:N	1:F:143:PRO:CD	2.77	0.47
1:F:275:THR:CG2	1:F:276:GLY:N	2.78	0.47
1:A:373:THR:HG22	1:A:374:HIS:CD2	2.50	0.47
1:C:7:LYS:HD3	1:C:111:TRP:HZ3	1.80	0.47
1:D:120:LYS:H	1:D:120:LYS:CD	2.28	0.47
1:D:54:HIS:H	1:D:54:HIS:CD2	2.32	0.47
1:E:48:ARG:HD2	1:E:119:PHE:HB2	1.95	0.47
1:G:379:PRO:O	1:G:383:HIS:HE1	1.98	0.47
1:H:105:THR:OG1	1:H:108:GLU:HG2	2.15	0.47
1:B:63:ILE:HG23	1:B:73:VAL:HG21	1.97	0.47
1:E:379:PRO:O	1:E:383:HIS:HE1	1.98	0.47
1:A:53:LEU:HG	1:A:130:ASP:HB2	1.96	0.47
1:D:7:LYS:HD3	1:D:111:TRP:HZ3	1.80	0.47
1:G:54:HIS:H	1:G:54:HIS:CD2	2.33	0.47
1:B:152:ILE:HG13	1:B:174:VAL:HG22	1.97	0.46
1:A:196:GLU:OE1	1:C:210:ILE:N	2.49	0.46
1:C:53:LEU:O	1:C:54:HIS:C	2.53	0.46
1:D:142:HIS:HB3	1:D:145:LEU:CD1	2.44	0.46
1:D:53:LEU:HG	1:D:130:ASP:HB2	1.98	0.46
1:D:74:ARG:HG3	1:D:119:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:LYS:NZ	1:E:250:GLN:HE22	2.12	0.46
1:A:6:TYR:CD1	1:A:6:TYR:C	2.88	0.46
1:B:28:MET:HB3	1:B:358:SER:HB2	1.97	0.46
1:D:7:LYS:NZ	1:D:7:LYS:O	2.40	0.46
1:A:7:LYS:HD3	1:A:111:TRP:HZ3	1.81	0.46
1:A:142:HIS:N	1:A:143:PRO:CD	2.78	0.46
1:C:419:PRO:HB2	1:C:422:GLY:N	2.29	0.46
1:D:48:ARG:HD2	1:D:119:PHE:CB	2.44	0.46
1:E:142:HIS:N	1:E:143:PRO:CD	2.79	0.46
1:H:307:VAL:H	1:H:308:LYS:NZ	2.14	0.46
1:A:194:CYS:SG	1:A:223:VAL:HG13	2.56	0.46
1:C:377:LYS:HD2	1:C:378:TYR:CE1	2.50	0.46
1:D:361:PHE:O	1:D:365:VAL:HG23	2.15	0.46
1:E:53:LEU:O	1:E:54:HIS:C	2.54	0.46
1:F:48:ARG:HD2	1:F:119:PHE:CB	2.46	0.46
1:G:6:TYR:OH	1:G:11:ILE:HD13	2.16	0.46
1:H:134:LEU:O	1:H:138:ILE:HG12	2.15	0.46
1:H:142:HIS:N	1:H:143:PRO:CD	2.78	0.46
1:H:53:LEU:O	1:H:54:HIS:C	2.54	0.46
1:A:31:LEU:HD13	1:A:61:VAL:HG12	1.97	0.46
1:B:172:LEU:HD22	1:B:174:VAL:H	1.80	0.46
1:B:373:THR:HG22	1:B:374:HIS:CD2	2.50	0.46
1:C:275:THR:HB	1:C:304:GLU:OE1	2.15	0.46
1:D:48:ARG:HD2	1:D:119:PHE:HB2	1.97	0.46
1:E:158:THR:O	1:E:161:HIS:HB3	2.16	0.46
1:E:181:ASP:HB2	1:E:384:PHE:HE1	1.80	0.46
1:F:57:VAL:H	1:F:84:GLN:NE2	2.14	0.46
1:G:7:LYS:CD	1:G:101:TRP:HZ3	2.29	0.46
1:G:4:LEU:HD13	1:G:99:PHE:HE1	1.81	0.46
1:H:124:LEU:HD23	1:H:124:LEU:N	2.30	0.46
1:C:243:ILE:HG21	1:D:408:LEU:CD1	2.45	0.46
1:C:91:ILE:HG23	1:C:96:ILE:HB	1.96	0.46
1:D:158:THR:O	1:D:161:HIS:HB3	2.15	0.46
1:E:161:HIS:NE2	1:E:165:LYS:NZ	2.55	0.46
1:E:7:LYS:O	1:E:7:LYS:NZ	2.41	0.46
1:F:361:PHE:O	1:F:365:VAL:HG23	2.16	0.46
1:H:31:LEU:HD13	1:H:61:VAL:HG12	1.97	0.46
1:B:142:HIS:HB3	1:B:145:LEU:CD1	2.44	0.46
1:D:101:TRP:CE2	1:D:104:GLU:HG2	2.51	0.46
1:D:57:VAL:H	1:D:84:GLN:NE2	2.13	0.46
1:E:364:GLN:HE21	1:E:364:GLN:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:HIS:CB	1:F:145:LEU:HD12	2.46	0.46
1:G:407:LYS:HE2	1:G:420:ILE:HG22	1.97	0.46
1:B:152:ILE:HD11	1:B:174:VAL:HG13	1.98	0.46
1:D:377:LYS:HD2	1:D:378:TYR:CE1	2.50	0.46
1:F:181:ASP:HB2	1:F:384:PHE:HE1	1.80	0.46
1:F:63:ILE:HG23	1:F:73:VAL:HG21	1.98	0.46
1:H:7:LYS:HZ1	1:H:100:ALA:CA	2.28	0.46
1:B:387:LYS:HE2	1:B:425:LYS:HB2	1.98	0.46
1:E:6:TYR:C	1:E:6:TYR:CD1	2.89	0.46
1:F:7:LYS:HE3	1:F:99:PHE:CA	2.45	0.46
1:G:247:ASN:HD21	1:H:425:LYS:HE2	1.81	0.46
1:G:35:ARG:NH2	1:G:64:GLU:HB2	2.31	0.46
1:G:7:LYS:HE3	1:G:99:PHE:CA	2.46	0.46
1:A:120:LYS:H	1:A:120:LYS:CD	2.29	0.46
1:B:121:ASP:OD1	1:B:121:ASP:N	2.48	0.46
1:B:45:LYS:O	1:B:45:LYS:HG3	2.13	0.46
1:B:54:HIS:HA	1:B:77:SER:OG	2.15	0.46
1:E:54:HIS:CD2	1:E:54:HIS:H	2.32	0.46
1:H:110:LEU:HD22	1:H:110:LEU:O	2.16	0.46
1:H:161:HIS:CD2	1:H:165:LYS:HZ1	2.32	0.46
1:H:57:VAL:H	1:H:84:GLN:NE2	2.14	0.46
1:A:300:HIS:HB2	2:A:432:NAD:O2D	2.15	0.45
1:B:7:LYS:CE	1:B:101:TRP:CZ3	2.99	0.45
1:D:53:LEU:O	1:D:54:HIS:C	2.54	0.45
1:G:167:MET:SD	1:G:381:GLY:HA2	2.56	0.45
1:G:424:PHE:C	1:G:425:LYS:HG2	2.35	0.45
1:B:111:TRP:O	1:B:115:GLN:HG2	2.17	0.45
1:B:38:TYR:HB3	1:B:43:PRO:CD	2.46	0.45
1:E:277:CYS:SG	1:F:412:GLN:HG2	2.56	0.45
1:E:17:GLY:HA3	1:E:86:HIS:O	2.17	0.45
1:F:196:GLU:HG2	1:H:203:LYS:HZ1	1.81	0.45
1:G:171:ILE:O	1:G:173:LYS:HG2	2.16	0.45
1:G:188:PHE:O	1:G:192:TYR:HB2	2.16	0.45
1:G:425:LYS:HE2	1:H:247:ASN:HD21	1.81	0.45
1:H:142:HIS:HB3	1:H:145:LEU:CD1	2.45	0.45
1:A:379:PRO:O	1:A:383:HIS:HE1	1.99	0.45
1:B:56:THR:HB	1:B:84:GLN:NE2	2.30	0.45
1:B:4:LEU:HD13	1:B:99:PHE:HE1	1.81	0.45
1:C:275:THR:CG2	1:C:276:GLY:N	2.79	0.45
1:H:4:LEU:CD1	1:H:4:LEU:H	2.27	0.45
1:H:6:TYR:CD1	1:H:6:TYR:C	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:O	1:B:138:ILE:HG12	2.17	0.45
1:C:158:THR:O	1:C:161:HIS:HB3	2.16	0.45
1:E:129:ASP:OD2	1:E:135:THR:CG2	2.65	0.45
1:F:7:LYS:HG2	1:F:111:TRP:CH2	2.52	0.45
1:G:307:VAL:H	1:G:308:LYS:NZ	2.15	0.45
1:H:54:HIS:HA	1:H:77:SER:OG	2.16	0.45
1:C:188:PHE:O	1:C:192:TYR:HB2	2.16	0.45
1:D:152:ILE:HG13	1:D:174:VAL:HG22	1.97	0.45
1:D:7:LYS:HE3	1:D:99:PHE:CA	2.46	0.45
1:E:151:GLY:HA3	1:E:371:LEU:HG	1.97	0.45
1:G:197:SER:OG	1:G:352:HIS:HD2	2.00	0.45
1:F:210:ILE:N	1:H:196:GLU:OE1	2.48	0.45
1:H:151:GLY:HA3	1:H:371:LEU:HG	1.98	0.45
1:A:57:VAL:H	1:A:84:GLN:NE2	2.15	0.45
1:D:189:ASP:OD1	1:D:189:ASP:C	2.55	0.45
1:F:364:GLN:HE21	1:F:364:GLN:HA	1.81	0.45
1:F:38:TYR:HB3	1:F:43:PRO:CD	2.46	0.45
1:G:300:HIS:CA	1:G:343:LEU:HD11	2.47	0.45
1:G:387:LYS:HE2	1:G:425:LYS:HB2	1.99	0.45
1:H:120:LYS:CD	1:H:120:LYS:H	2.28	0.45
1:H:38:TYR:HB3	1:H:43:PRO:CD	2.46	0.45
1:A:246:ILE:O	1:A:250:GLN:HG3	2.17	0.45
1:D:188:PHE:O	1:D:192:TYR:HB2	2.16	0.45
1:D:4:LEU:H	1:D:4:LEU:CD1	2.29	0.45
1:D:35:ARG:NH2	1:D:64:GLU:HB2	2.32	0.45
1:F:300:HIS:CA	1:F:343:LEU:HD11	2.46	0.45
1:F:45:LYS:HA	1:F:70:GLY:O	2.16	0.45
1:G:101:TRP:HZ2	1:G:108:GLU:CD	2.20	0.45
1:H:343:LEU:HG	2:H:432:NAD:H71N	1.82	0.45
1:H:45:LYS:O	1:H:45:LYS:HG3	2.17	0.45
1:A:158:THR:O	1:A:161:HIS:HB3	2.17	0.45
1:A:4:LEU:HD13	1:A:99:PHE:HE1	1.81	0.45
1:C:142:HIS:HB3	1:C:145:LEU:CD1	2.46	0.45
1:C:197:SER:OG	1:C:352:HIS:HD2	2.00	0.45
1:D:300:HIS:CA	1:D:343:LEU:HD11	2.47	0.45
1:E:277:CYS:HA	1:F:415:TYR:CE2	2.51	0.45
1:F:152:ILE:HG22	1:F:153:SER:N	2.31	0.45
1:F:6:TYR:CD1	1:F:6:TYR:C	2.90	0.45
1:H:158:THR:O	1:H:161:HIS:HB3	2.16	0.45
1:H:74:ARG:HE	1:H:120:LYS:HZ1	1.64	0.45
1:H:7:LYS:NZ	1:H:7:LYS:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93:LYS:HG3	1:H:93:LYS:O	2.16	0.45
1:A:110:LEU:O	1:A:110:LEU:HD22	2.17	0.45
1:B:101:TRP:HZ2	1:B:108:GLU:CD	2.20	0.45
1:B:209:MET:HB2	1:D:353:PRO:CB	2.47	0.45
1:B:7:LYS:CD	1:B:101:TRP:HZ3	2.30	0.45
1:C:177:ILE:HG13	1:C:371:LEU:HD21	1.99	0.45
1:C:247:ASN:HD21	1:D:425:LYS:HE2	1.82	0.45
1:D:17:GLY:HA3	1:D:86:HIS:O	2.16	0.45
1:F:165:LYS:HE3	1:F:165:LYS:HB2	1.67	0.45
1:G:101:TRP:HZ2	1:G:108:GLU:OE1	2.00	0.45
1:H:44:LEU:HB3	1:H:71:ALA:HB2	1.98	0.45
1:B:171:ILE:O	1:B:173:LYS:HG2	2.17	0.45
1:C:387:LYS:HE2	1:C:425:LYS:HB2	1.99	0.45
1:C:7:LYS:HE3	1:C:99:PHE:CA	2.47	0.45
1:D:81:PHE:O	1:D:102:LYS:HE2	2.17	0.45
1:D:373:THR:HG22	1:D:374:HIS:CD2	2.52	0.45
1:E:184:THR:HA	1:E:188:PHE:CD1	2.52	0.45
1:G:206:THR:O	1:G:207:ASP:HB2	2.16	0.45
1:G:364:GLN:HE21	1:G:364:GLN:HA	1.82	0.45
1:H:121:ASP:OD1	1:H:121:ASP:N	2.47	0.45
1:C:189:ASP:C	1:C:189:ASP:OD1	2.55	0.44
1:D:246:ILE:O	1:D:250:GLN:HG3	2.17	0.44
1:D:364:GLN:HE21	1:D:364:GLN:HA	1.81	0.44
1:E:161:HIS:CD2	1:E:165:LYS:HZ1	2.35	0.44
1:E:4:LEU:HD13	1:E:99:PHE:HE1	1.82	0.44
1:A:161:HIS:CD2	1:A:165:LYS:HZ1	2.35	0.44
1:A:38:TYR:HB3	1:A:43:PRO:CD	2.47	0.44
1:B:151:GLY:HA3	1:B:371:LEU:HG	2.00	0.44
1:C:161:HIS:NE2	1:C:165:LYS:NZ	2.54	0.44
1:E:7:LYS:HZ1	1:E:100:ALA:CA	2.30	0.44
1:F:54:HIS:CD2	1:F:54:HIS:H	2.34	0.44
1:G:409:THR:H	1:G:412:GLN:NE2	2.09	0.44
1:G:31:LEU:HD13	1:G:61:VAL:HG12	1.99	0.44
1:B:308:LYS:HD2	1:B:308:LYS:N	2.18	0.44
1:D:101:TRP:HZ2	1:D:108:GLU:OE1	2.00	0.44
1:E:7:LYS:CD	1:E:101:TRP:HZ3	2.31	0.44
1:E:275:THR:HB	1:E:304:GLU:OE1	2.17	0.44
1:E:364:GLN:HE21	1:E:364:GLN:CA	2.30	0.44
1:F:364:GLN:HE21	1:F:364:GLN:CA	2.31	0.44
1:G:419:PRO:CG	1:G:422:GLY:HA3	2.45	0.44
1:G:426:PRO:HB2	1:G:428:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:HIS:CA	1:A:343:LEU:HD11	2.47	0.44
1:B:10:ASP:HB3	1:B:13:LEU:HD22	2.00	0.44
1:B:165:LYS:HB2	1:B:165:LYS:HE3	1.73	0.44
1:C:152:ILE:HG13	1:C:174:VAL:HG22	2.00	0.44
1:C:321:LYS:HB2	1:C:322:PRO:HD2	2.00	0.44
1:D:300:HIS:HB2	2:D:432:NAD:O2D	2.17	0.44
1:E:152:ILE:HG13	1:E:174:VAL:HG22	1.98	0.44
1:E:373:THR:HG22	1:E:374:HIS:CD2	2.52	0.44
1:E:38:TYR:HB3	1:E:43:PRO:CD	2.47	0.44
1:F:110:LEU:O	1:F:110:LEU:HD22	2.17	0.44
1:G:74:ARG:HE	1:G:120:LYS:HZ3	1.64	0.44
1:A:152:ILE:HG22	1:A:153:SER:N	2.33	0.44
1:B:206:THR:O	1:B:207:ASP:HB2	2.17	0.44
1:B:300:HIS:CA	1:B:343:LEU:HD11	2.47	0.44
1:C:7:LYS:CE	1:C:101:TRP:CZ3	3.01	0.44
1:C:155:GLU:O	1:C:180:ASN:HB2	2.18	0.44
1:C:38:TYR:HB3	1:C:43:PRO:CD	2.48	0.44
1:G:7:LYS:O	1:G:7:LYS:NZ	2.40	0.44
1:H:300:HIS:CA	1:H:343:LEU:HD11	2.48	0.44
1:H:2:ASP:HB3	1:H:3:LYS:H	1.60	0.44
1:A:134:LEU:O	1:A:138:ILE:HG12	2.18	0.44
1:A:184:THR:HA	1:A:188:PHE:CD1	2.52	0.44
1:A:53:LEU:O	1:A:54:HIS:C	2.55	0.44
1:B:155:GLU:O	1:B:180:ASN:HB2	2.18	0.44
1:B:44:LEU:HB3	1:B:71:ALA:HB2	1.99	0.44
1:C:17:GLY:HA3	1:C:86:HIS:O	2.18	0.44
1:D:119:PHE:HB2	1:D:122:GLY:O	2.18	0.44
1:E:110:LEU:HD22	1:E:110:LEU:O	2.17	0.44
1:E:142:HIS:HB3	1:E:145:LEU:CD1	2.47	0.44
1:H:194:CYS:SG	1:H:223:VAL:HG13	2.58	0.44
1:H:210:ILE:HG22	1:H:236:ALA:HB2	2.00	0.44
1:A:275:THR:CG2	1:A:276:GLY:N	2.81	0.44
1:A:361:PHE:O	1:A:365:VAL:HG23	2.17	0.44
1:A:419:PRO:CG	1:A:422:GLY:HA3	2.44	0.44
1:C:329:LEU:HB2	1:C:331:ASN:OD1	2.17	0.44
1:F:53:LEU:HG	1:F:130:ASP:HB2	2.00	0.44
1:G:19:LYS:HE3	4:G:464:HOH:O	2.18	0.44
1:G:6:TYR:C	1:G:6:TYR:CD1	2.91	0.44
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.85	0.44
1:C:138:ILE:HG22	1:C:146:LEU:CD1	2.48	0.44
1:F:26:ASN:HD22	1:F:26:ASN:HA	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:CYS:HA	1:F:415:TYR:HE2	1.82	0.44
1:G:154:GLU:HG3	1:G:160:VAL:HG23	2.00	0.44
1:H:172:LEU:HD22	1:H:174:VAL:H	1.82	0.44
1:H:35:ARG:NH2	1:H:64:GLU:HB2	2.33	0.44
1:H:4:LEU:HD13	1:H:99:PHE:HE1	1.81	0.44
1:A:93:LYS:O	1:A:93:LYS:HG3	2.17	0.44
1:C:300:HIS:HB2	2:C:432:NAD:O2D	2.18	0.44
1:C:310:LEU:HA	1:C:310:LEU:HD23	1.89	0.44
1:D:63:ILE:HG23	1:D:73:VAL:HG21	2.00	0.44
1:E:155:GLU:O	1:E:180:ASN:HB2	2.18	0.44
1:E:63:ILE:HG23	1:E:73:VAL:HG21	1.99	0.44
1:F:124:LEU:HD23	1:F:124:LEU:N	2.33	0.44
1:G:57:VAL:H	1:G:84:GLN:NE2	2.16	0.44
1:G:91:ILE:HG23	1:G:96:ILE:HB	1.99	0.44
1:A:215:ALA:HB1	1:A:231:LEU:HD13	2.00	0.43
1:B:101:TRP:HZ2	1:B:108:GLU:OE1	2.00	0.43
1:B:110:LEU:HD22	1:B:110:LEU:O	2.18	0.43
1:D:7:LYS:HG2	1:D:111:TRP:CZ3	2.53	0.43
1:D:321:LYS:HB2	1:D:322:PRO:HD2	1.99	0.43
1:F:188:PHE:O	1:F:192:TYR:HB2	2.18	0.43
1:F:215:ALA:HB1	1:F:231:LEU:HD13	2.00	0.43
1:F:343:LEU:HG	2:F:432:NAD:H71N	1.81	0.43
1:G:167:MET:HG2	1:G:172:LEU:HD12	1.99	0.43
1:H:152:ILE:HD11	1:H:174:VAL:HG13	1.98	0.43
1:H:197:SER:OG	1:H:352:HIS:HD2	2.01	0.43
1:H:24:ALA:O	1:H:28:MET:HG3	2.18	0.43
1:A:101:TRP:HZ2	1:A:108:GLU:CD	2.22	0.43
1:A:189:ASP:C	1:A:189:ASP:OD1	2.56	0.43
1:D:4:LEU:HD13	1:D:99:PHE:HE1	1.82	0.43
1:H:355:PHE:CZ	1:H:397:HIS:HB3	2.53	0.43
1:A:7:LYS:CD	1:A:101:TRP:HZ3	2.32	0.43
1:A:54:HIS:CD2	1:A:54:HIS:H	2.36	0.43
1:A:7:LYS:CE	1:A:101:TRP:CZ3	3.02	0.43
1:B:158:THR:O	1:B:161:HIS:HB3	2.18	0.43
1:B:425:LYS:HD2	1:B:429:TYR:CD2	2.54	0.43
1:C:206:THR:O	1:C:207:ASP:HB2	2.18	0.43
1:C:387:LYS:O	1:C:391:GLU:HG3	2.18	0.43
1:G:300:HIS:HB2	2:G:432:NAD:O2D	2.18	0.43
1:B:160:VAL:HG11	1:B:178:ASN:ND2	2.33	0.43
1:B:55:MET:HB3	1:B:83:THR:HG23	1.99	0.43
1:D:93:LYS:O	1:D:93:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:LYS:CE	1:E:101:TRP:CZ3	3.01	0.43
1:E:74:ARG:HE	1:E:120:LYS:HZ3	1.65	0.43
1:F:132:GLY:O	1:F:136:ASN:HB2	2.18	0.43
1:F:158:THR:O	1:F:161:HIS:HB3	2.18	0.43
1:F:196:GLU:OE1	1:H:210:ILE:N	2.49	0.43
1:G:10:ASP:HB3	1:G:13:LEU:HD22	2.01	0.43
1:G:172:LEU:HD22	1:G:174:VAL:H	1.84	0.43
1:G:277:CYS:HA	1:H:415:TYR:CE2	2.54	0.43
1:H:203:LYS:O	1:H:207:ASP:N	2.50	0.43
1:B:101:TRP:CE2	1:B:104:GLU:HG2	2.54	0.43
1:B:155:GLU:HB3	1:B:364:GLN:OE1	2.18	0.43
1:C:101:TRP:HZ2	1:C:108:GLU:CD	2.21	0.43
1:D:275:THR:HB	1:D:304:GLU:OE1	2.19	0.43
1:E:425:LYS:HE2	1:F:247:ASN:HD21	1.84	0.43
1:E:7:LYS:HG2	1:E:111:TRP:CH2	2.54	0.43
1:F:419:PRO:CG	1:F:422:GLY:HA3	2.42	0.43
1:G:53:LEU:HG	1:G:130:ASP:HB2	2.01	0.43
1:G:321:LYS:HB2	1:G:322:PRO:HD2	2.01	0.43
1:H:7:LYS:HG2	1:H:111:TRP:CH2	2.54	0.43
1:H:208:VAL:HG22	1:H:209:MET:N	2.33	0.43
1:H:275:THR:CG2	1:H:276:GLY:N	2.81	0.43
1:H:387:LYS:HE2	1:H:425:LYS:HB2	2.00	0.43
1:B:409:THR:H	1:B:412:GLN:NE2	2.09	0.43
1:C:56:THR:HB	1:C:84:GLN:NE2	2.34	0.43
1:E:101:TRP:HZ2	1:E:108:GLU:OE1	2.01	0.43
1:F:111:TRP:O	1:F:115:GLN:HG2	2.19	0.43
1:F:7:LYS:CE	1:F:101:TRP:CZ3	3.02	0.43
1:G:7:LYS:HG2	1:G:111:TRP:CH2	2.53	0.43
1:A:343:LEU:HG	2:A:432:NAD:H71N	1.83	0.43
1:B:210:ILE:HG22	1:B:236:ALA:HB2	2.01	0.43
1:B:345:ASN:O	1:B:349:ALA:HB3	2.18	0.43
1:C:198:LEU:HD22	1:C:227:CYS:SG	2.59	0.43
1:E:55:MET:HB3	1:E:83:THR:HG23	2.01	0.43
1:F:35:ARG:NH2	1:F:64:GLU:HB2	2.33	0.43
1:G:153:SER:HB2	1:G:368:GLN:HE21	1.84	0.43
1:H:275:THR:HB	1:H:304:GLU:OE1	2.19	0.43
1:H:419:PRO:CG	1:H:422:GLY:HA3	2.48	0.43
1:A:26:ASN:HD22	1:A:26:ASN:HA	1.64	0.43
1:C:31:LEU:HD13	1:C:61:VAL:HG12	2.00	0.43
1:D:37:MET:HE2	1:D:38:TYR:CE2	2.53	0.43
1:E:329:LEU:HB2	1:E:331:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:LEU:HD22	1:G:7:LYS:HB3	2.01	0.43
1:H:373:THR:HG22	1:H:374:HIS:CD2	2.53	0.43
1:H:7:LYS:CE	1:H:101:TRP:CZ3	3.02	0.43
1:A:277:CYS:HB3	1:B:416:LEU:CD2	2.45	0.43
1:B:6:TYR:OH	1:B:11:ILE:HD13	2.18	0.43
1:D:56:THR:HB	1:D:84:GLN:NE2	2.33	0.43
1:E:165:LYS:HE3	1:E:165:LYS:HB2	1.69	0.43
1:E:203:LYS:O	1:E:207:ASP:N	2.51	0.43
1:F:4:LEU:HD11	1:F:111:TRP:HH2	1.84	0.43
1:G:134:LEU:O	1:G:138:ILE:HG12	2.18	0.43
1:A:121:ASP:N	1:A:121:ASP:OD1	2.48	0.43
1:B:7:LYS:HG2	1:B:111:TRP:CH2	2.53	0.43
1:B:275:THR:CG2	1:B:276:GLY:N	2.82	0.43
1:B:91:ILE:HD13	1:B:91:ILE:HA	1.86	0.43
1:D:7:LYS:HG2	1:D:111:TRP:CH2	2.53	0.43
1:D:45:LYS:HA	1:D:70:GLY:O	2.18	0.43
1:F:172:LEU:HD22	1:F:174:VAL:H	1.84	0.43
1:G:119:PHE:HB2	1:G:122:GLY:O	2.19	0.43
1:F:237:ARG:NE	1:G:257:GLU:HB2	2.34	0.43
1:A:210:ILE:N	1:C:196:GLU:OE1	2.52	0.42
1:A:153:SER:HB2	1:A:368:GLN:HE21	1.83	0.42
1:C:132:GLY:O	1:C:136:ASN:HB2	2.19	0.42
1:E:121:ASP:N	1:E:121:ASP:OD1	2.47	0.42
1:E:196:GLU:OE1	1:G:210:ILE:N	2.47	0.42
1:E:6:TYR:OH	1:E:11:ILE:HD13	2.19	0.42
1:F:101:TRP:HZ2	1:F:108:GLU:OE1	2.02	0.42
1:F:161:HIS:NE2	1:F:165:LYS:NZ	2.57	0.42
1:G:161:HIS:CD2	1:G:165:LYS:HZ1	2.37	0.42
1:H:419:PRO:HB2	1:H:422:GLY:N	2.32	0.42
1:C:9:ALA:HB2	1:C:101:TRP:HB2	2.01	0.42
1:C:424:PHE:C	1:C:425:LYS:HG2	2.39	0.42
1:D:206:THR:O	1:D:207:ASP:HB2	2.19	0.42
1:D:364:GLN:CA	1:D:364:GLN:HE21	2.31	0.42
1:D:387:LYS:HE2	1:D:425:LYS:HB2	2.00	0.42
1:E:187:LYS:HE2	4:F:457:HOH:O	2.19	0.42
1:E:323:GLN:HG3	1:E:339:ALA:HA	2.01	0.42
1:F:177:ILE:HG13	1:F:371:LEU:HD21	2.01	0.42
1:F:206:THR:O	1:F:207:ASP:HB2	2.20	0.42
1:G:55:MET:HB3	1:G:83:THR:HG23	2.00	0.42
1:H:152:ILE:HG13	1:H:174:VAL:HG22	2.01	0.42
1:H:26:ASN:HD22	1:H:26:ASN:HA	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TRP:HZ2	1:A:108:GLU:OE1	2.02	0.42
1:A:152:ILE:HG13	1:A:174:VAL:HG22	2.02	0.42
1:A:277:CYS:O	1:A:304:GLU:HG2	2.19	0.42
1:A:44:LEU:HB3	1:A:71:ALA:HB2	2.00	0.42
1:B:7:LYS:HG2	1:B:111:TRP:CZ3	2.54	0.42
1:B:53:LEU:O	1:B:54:HIS:C	2.56	0.42
1:C:2:ASP:HB3	1:C:3:LYS:H	1.61	0.42
1:C:4:LEU:HD11	1:C:111:TRP:HH2	1.81	0.42
1:E:215:ALA:HB1	1:E:231:LEU:HD13	2.01	0.42
1:F:321:LYS:HB2	1:F:322:PRO:HD2	2.00	0.42
1:G:153:SER:HB2	1:G:368:GLN:NE2	2.34	0.42
1:F:257:GLU:HB2	1:G:237:ARG:NE	2.34	0.42
1:H:124:LEU:HD23	1:H:124:LEU:H	1.84	0.42
1:H:155:GLU:O	1:H:180:ASN:HB2	2.20	0.42
1:H:425:LYS:HD2	1:H:429:TYR:CD2	2.54	0.42
1:A:403:VAL:HG13	1:B:258:VAL:HB	2.02	0.42
1:B:74:ARG:HE	1:B:120:LYS:HZ1	1.66	0.42
1:D:101:TRP:HZ2	1:D:108:GLU:CD	2.23	0.42
1:D:31:LEU:HD13	1:D:61:VAL:HG12	2.01	0.42
1:F:10:ASP:HB3	1:F:13:LEU:HD22	2.00	0.42
1:E:353:PRO:CB	1:G:209:MET:HB2	2.47	0.42
1:G:210:ILE:HG22	1:G:236:ALA:HB2	2.00	0.42
1:G:7:LYS:CE	1:G:101:TRP:CZ3	3.01	0.42
1:H:3:LYS:HE2	1:H:115:GLN:NE2	2.34	0.42
1:A:133:ASP:HB2	4:A:476:HOH:O	2.19	0.42
1:B:4:LEU:HD22	1:B:7:LYS:HB3	2.00	0.42
1:E:377:LYS:HD2	1:E:378:TYR:CE1	2.54	0.42
1:F:7:LYS:CD	1:F:101:TRP:HZ3	2.31	0.42
1:G:203:LYS:O	1:G:207:ASP:N	2.52	0.42
1:B:329:LEU:HB2	1:B:331:ASN:OD1	2.20	0.42
1:B:7:LYS:NZ	1:B:7:LYS:O	2.41	0.42
1:C:110:LEU:HD22	1:C:110:LEU:O	2.19	0.42
1:C:53:LEU:HG	1:C:130:ASP:HB2	2.01	0.42
1:D:2:ASP:HB3	1:D:3:LYS:H	1.63	0.42
1:E:53:LEU:HG	1:E:130:ASP:HB2	2.01	0.42
1:E:198:LEU:HD22	1:E:227:CYS:SG	2.59	0.42
1:F:119:PHE:HB3	1:F:120:LYS:HE2	2.02	0.42
1:H:53:LEU:HG	1:H:130:ASP:HB2	2.02	0.42
1:G:415:TYR:OH	1:H:303:VAL:HG21	2.20	0.42
1:B:31:LEU:HD13	1:B:61:VAL:HG12	2.01	0.42
1:C:119:PHE:HB2	1:C:122:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD23	1:C:124:LEU:N	2.35	0.42
1:B:210:ILE:N	1:D:196:GLU:OE1	2.50	0.42
1:E:119:PHE:HB2	1:E:122:GLY:O	2.20	0.42
1:E:183:VAL:HG23	1:E:390:ASP:OD2	2.20	0.42
1:E:74:ARG:HE	1:E:120:LYS:HZ1	1.66	0.42
1:F:167:MET:SD	1:F:381:GLY:HA2	2.60	0.42
1:F:408:LEU:HA	1:F:408:LEU:HD12	1.88	0.42
1:G:184:THR:HA	1:G:188:PHE:CD1	2.54	0.42
1:G:329:LEU:HB2	1:G:331:ASN:OD1	2.19	0.42
1:H:6:TYR:OH	1:H:11:ILE:HD13	2.19	0.42
1:H:153:SER:HB2	1:H:368:GLN:HE21	1.84	0.42
1:H:184:THR:HA	1:H:188:PHE:CD1	2.55	0.42
1:A:150:ARG:HD2	1:A:372:TRP:CE3	2.55	0.42
1:C:184:THR:HA	1:C:188:PHE:CD1	2.55	0.42
1:C:210:ILE:HG22	1:C:236:ALA:HB2	2.01	0.42
1:D:105:THR:HG23	1:D:108:GLU:OE1	2.19	0.42
1:D:329:LEU:HB2	1:D:331:ASN:OD1	2.20	0.42
1:E:188:PHE:O	1:E:192:TYR:HB2	2.20	0.42
1:E:419:PRO:HB2	1:E:422:GLY:N	2.32	0.42
1:E:44:LEU:HB3	1:E:71:ALA:HB2	2.00	0.42
1:F:7:LYS:HG2	1:F:111:TRP:CZ3	2.55	0.42
1:F:210:ILE:HG22	1:F:236:ALA:HB2	2.01	0.42
1:F:44:LEU:HB3	1:F:71:ALA:HB2	2.01	0.42
1:G:355:PHE:CZ	1:G:397:HIS:HB3	2.55	0.42
1:G:277:CYS:HA	1:H:415:TYR:HE2	1.84	0.42
1:A:364:GLN:HA	1:A:364:GLN:HE21	1.85	0.42
1:A:409:THR:H	1:A:412:GLN:NE2	2.10	0.42
1:B:300:HIS:HB2	2:B:432:NAD:O2D	2.19	0.42
1:B:45:LYS:HA	1:B:70:GLY:O	2.20	0.42
1:B:4:LEU:HD11	1:B:111:TRP:HH2	1.83	0.42
1:C:153:SER:HB2	1:C:368:GLN:HE21	1.85	0.42
1:C:45:LYS:HA	1:C:70:GLY:O	2.19	0.42
1:D:155:GLU:O	1:D:180:ASN:HB2	2.20	0.42
1:D:184:THR:HA	1:D:188:PHE:CD1	2.54	0.42
1:D:38:TYR:HB3	1:D:43:PRO:CD	2.49	0.42
1:D:4:LEU:HD22	1:D:7:LYS:HB3	2.01	0.42
1:D:91:ILE:HA	1:D:91:ILE:HD13	1.84	0.42
1:E:387:LYS:HE2	1:E:425:LYS:HB2	2.02	0.42
1:F:53:LEU:O	1:F:54:HIS:C	2.58	0.42
1:F:55:MET:HB3	1:F:83:THR:HG23	2.01	0.42
1:G:142:HIS:HB3	1:G:145:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:THR:HB	1:G:304:GLU:OE1	2.19	0.42
1:G:17:GLY:HA3	1:G:86:HIS:O	2.20	0.42
1:H:150:ARG:HD2	1:H:372:TRP:CE3	2.55	0.42
1:H:160:VAL:HG11	1:H:178:ASN:ND2	2.34	0.42
1:H:49:ILE:HD12	1:H:71:ALA:HB1	2.02	0.42
1:A:321:LYS:HB2	1:A:322:PRO:HD2	2.01	0.42
1:A:63:ILE:HG23	1:A:73:VAL:HG21	2.01	0.42
1:B:105:THR:HG23	1:B:108:GLU:OE1	2.19	0.42
1:C:7:LYS:HG2	1:C:111:TRP:CZ3	2.55	0.42
1:D:153:SER:HB2	1:D:368:GLN:HE21	1.85	0.42
1:E:171:ILE:O	1:E:173:LYS:HG2	2.20	0.42
1:G:7:LYS:HG2	1:G:111:TRP:CZ3	2.55	0.42
1:G:124:LEU:HD23	1:G:124:LEU:N	2.34	0.42
1:G:3:LYS:HE2	1:G:115:GLN:NE2	2.33	0.42
1:A:102:LYS:HE3	4:A:469:HOH:O	2.19	0.41
1:B:53:LEU:HG	1:B:130:ASP:HB2	2.02	0.41
1:B:419:PRO:CG	1:B:422:GLY:HA3	2.45	0.41
1:C:7:LYS:HG2	1:C:111:TRP:CH2	2.54	0.41
1:D:167:MET:HG2	1:D:172:LEU:HD12	2.02	0.41
1:F:355:PHE:CZ	1:F:397:HIS:HB3	2.55	0.41
1:F:57:VAL:HG23	1:F:84:GLN:HE21	1.84	0.41
1:G:415:TYR:CE2	1:H:277:CYS:HA	2.55	0.41
1:H:7:LYS:CD	1:H:101:TRP:HZ3	2.33	0.41
1:H:101:TRP:HZ2	1:H:108:GLU:CD	2.23	0.41
1:H:129:ASP:OD2	1:H:135:THR:CG2	2.66	0.41
1:A:142:HIS:HB3	1:A:145:LEU:CD1	2.49	0.41
1:B:139:HIS:ND1	1:B:146:LEU:HD11	2.35	0.41
1:C:101:TRP:HZ2	1:C:108:GLU:OE1	2.03	0.41
1:E:206:THR:O	1:E:207:ASP:HB2	2.20	0.41
1:E:343:LEU:HG	2:E:432:NAD:H71N	1.84	0.41
1:E:424:PHE:C	1:E:425:LYS:HG2	2.39	0.41
1:F:151:GLY:HA3	1:F:371:LEU:HG	2.02	0.41
1:F:7:LYS:O	1:F:7:LYS:NZ	2.43	0.41
1:G:430:ARG:CZ	1:H:183:VAL:HG22	2.50	0.41
1:A:172:LEU:HD22	1:A:174:VAL:H	1.85	0.41
1:A:206:THR:O	1:A:207:ASP:HB2	2.20	0.41
1:A:45:LYS:HA	1:A:70:GLY:O	2.21	0.41
1:C:136:ASN:O	1:C:140:THR:HG23	2.21	0.41
1:C:172:LEU:HD22	1:C:174:VAL:H	1.85	0.41
1:C:180:ASN:O	1:C:186:SER:HB2	2.19	0.41
1:C:203:LYS:O	1:C:207:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ASP:HB3	1:D:13:LEU:HD22	2.01	0.41
1:F:17:GLY:HA3	1:F:86:HIS:O	2.19	0.41
1:F:424:PHE:C	1:F:425:LYS:HG2	2.41	0.41
1:G:364:GLN:HE21	1:G:364:GLN:CA	2.33	0.41
1:H:206:THR:O	1:H:207:ASP:HB2	2.20	0.41
1:H:215:ALA:HB1	1:H:231:LEU:HD13	2.02	0.41
1:H:329:LEU:HB2	1:H:331:ASN:OD1	2.20	0.41
1:H:364:GLN:HE21	1:H:364:GLN:HA	1.84	0.41
1:A:210:ILE:HG22	1:A:236:ALA:HB2	2.02	0.41
1:A:387:LYS:HE2	1:A:425:LYS:HB2	2.03	0.41
1:B:364:GLN:CA	1:B:364:GLN:HE21	2.33	0.41
1:C:426:PRO:HB2	1:C:428:HIS:CE1	2.55	0.41
1:D:113:ILE:CG2	1:D:137:LEU:HD22	2.51	0.41
1:G:4:LEU:HD11	1:G:111:TRP:HH2	1.83	0.41
1:B:119:PHE:HB2	1:B:122:GLY:O	2.20	0.41
1:A:408:LEU:CD1	1:B:243:ILE:HG21	2.41	0.41
1:E:120:LYS:H	1:E:120:LYS:CD	2.27	0.41
1:E:134:LEU:O	1:E:138:ILE:HG12	2.21	0.41
1:E:45:LYS:HA	1:E:70:GLY:O	2.20	0.41
1:F:139:HIS:ND1	1:F:146:LEU:HD11	2.36	0.41
1:F:198:LEU:HD22	1:F:227:CYS:SG	2.60	0.41
1:F:373:THR:HG22	1:F:374:HIS:CG	2.56	0.41
1:G:194:CYS:SG	1:G:223:VAL:HG13	2.61	0.41
1:G:343:LEU:HG	2:G:432:NAD:H71N	1.83	0.41
1:A:306:ASP:OD1	1:A:308:LYS:HD3	2.20	0.41
1:C:321:LYS:HB2	1:C:322:PRO:CD	2.51	0.41
1:C:4:LEU:HD22	1:C:7:LYS:HB3	2.03	0.41
1:D:152:ILE:HD11	1:D:174:VAL:HG13	2.02	0.41
1:D:345:ASN:O	1:D:349:ALA:HB3	2.20	0.41
1:D:373:THR:HG22	1:D:374:HIS:CG	2.56	0.41
1:D:385:LEU:HA	1:D:385:LEU:HD12	1.90	0.41
1:E:321:LYS:HB2	1:E:322:PRO:HD2	2.02	0.41
1:E:197:SER:OG	1:E:352:HIS:HD2	2.04	0.41
1:E:54:HIS:HA	1:E:77:SER:OG	2.21	0.41
1:F:124:LEU:HD23	1:F:124:LEU:H	1.86	0.41
1:G:158:THR:O	1:G:161:HIS:HB3	2.20	0.41
1:G:415:TYR:HE2	1:H:277:CYS:HA	1.85	0.41
1:H:27:GLU:O	1:H:29:PRO:HD3	2.21	0.41
1:H:63:ILE:HG23	1:H:73:VAL:HG21	2.02	0.41
1:A:275:THR:HB	1:A:304:GLU:OE1	2.21	0.41
1:D:124:LEU:N	1:D:124:LEU:HD23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:LYS:HB2	1:D:322:PRO:CD	2.51	0.41
1:E:183:VAL:HG21	1:E:431:TYR:CE1	2.55	0.41
1:F:154:GLU:OE1	1:F:156:THR:HG22	2.21	0.41
1:E:277:CYS:HB2	1:F:415:TYR:HD2	1.84	0.41
1:E:303:VAL:HG21	1:F:415:TYR:OH	2.20	0.41
1:H:138:ILE:HG22	1:H:146:LEU:CD1	2.50	0.41
1:H:165:LYS:HB2	1:H:165:LYS:HE3	1.71	0.41
1:H:388:LYS:HG2	1:H:423:PRO:HD3	2.02	0.41
1:A:155:GLU:O	1:A:180:ASN:HB2	2.21	0.41
1:A:160:VAL:HG11	1:A:178:ASN:ND2	2.34	0.41
1:A:54:HIS:HA	1:A:77:SER:OG	2.21	0.41
1:B:246:ILE:O	1:B:250:GLN:HG3	2.20	0.41
1:B:321:LYS:HB2	1:B:322:PRO:HD2	2.01	0.41
1:C:139:HIS:ND1	1:C:146:LEU:HD11	2.36	0.41
1:C:246:ILE:O	1:C:250:GLN:HG3	2.20	0.41
1:C:343:LEU:HG	2:C:432:NAD:H71N	1.82	0.41
1:D:323:GLN:HG3	1:D:339:ALA:HA	2.02	0.41
1:D:388:LYS:HG3	1:D:388:LYS:HZ3	1.79	0.41
1:D:4:LEU:HD11	1:D:111:TRP:HH2	1.79	0.41
1:D:7:LYS:CD	1:D:101:TRP:HZ3	2.33	0.41
1:D:9:ALA:HB2	1:D:101:TRP:HB2	2.02	0.41
1:E:101:TRP:HZ2	1:E:108:GLU:CD	2.24	0.41
1:G:155:GLU:HB3	1:G:364:GLN:OE1	2.20	0.41
1:G:38:TYR:HB3	1:G:43:PRO:CD	2.51	0.41
1:H:113:ILE:CG2	1:H:137:LEU:HD22	2.51	0.41
1:B:124:LEU:N	1:B:124:LEU:HD23	2.36	0.41
1:D:151:GLY:HA3	1:D:371:LEU:HG	2.02	0.41
1:B:196:GLU:OE1	1:D:209:MET:HG3	2.21	0.41
1:D:210:ILE:HG22	1:D:236:ALA:HB2	2.02	0.41
1:D:424:PHE:C	1:D:425:LYS:HG2	2.40	0.41
1:E:155:GLU:HB3	1:E:364:GLN:OE1	2.21	0.41
1:E:300:HIS:H	2:E:432:NAD:C1D	2.22	0.41
1:F:387:LYS:HE2	1:F:425:LYS:HB2	2.02	0.41
1:G:161:HIS:NE2	1:G:165:LYS:NZ	2.58	0.41
1:G:225:LYS:NZ	1:G:250:GLN:HE22	2.18	0.41
1:A:171:ILE:O	1:A:173:LYS:HG2	2.21	0.41
1:B:161:HIS:NE2	1:B:165:LYS:NZ	2.56	0.41
1:C:152:ILE:HD11	1:C:174:VAL:HG13	2.03	0.41
1:C:171:ILE:O	1:C:173:LYS:HG2	2.20	0.41
1:C:153:SER:HB2	1:C:368:GLN:NE2	2.35	0.41
1:D:187:LYS:HG2	4:D:434:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:MET:HG3	4:D:467:HOH:O	2.21	0.41
1:D:7:LYS:CE	1:D:101:TRP:CZ3	3.03	0.41
1:E:153:SER:HB2	1:E:368:GLN:NE2	2.36	0.41
1:E:385:LEU:HA	1:E:385:LEU:HD12	1.93	0.41
1:F:377:LYS:HD2	1:F:378:TYR:CE1	2.56	0.41
1:G:178:ASN:ND2	1:G:181:ASP:HB2	2.36	0.41
1:G:215:ALA:HB1	1:G:231:LEU:HD13	2.03	0.41
1:A:105:THR:HG23	1:A:108:GLU:OE1	2.20	0.41
1:A:155:GLU:HB3	1:A:364:GLN:OE1	2.21	0.41
1:A:153:SER:HB2	1:A:368:GLN:NE2	2.35	0.41
1:B:113:ILE:CG2	1:B:137:LEU:HD22	2.51	0.41
1:B:198:LEU:HD22	1:B:227:CYS:SG	2.61	0.41
1:B:215:ALA:HB1	1:B:231:LEU:HD13	2.02	0.41
1:B:300:HIS:H	2:B:432:NAD:C1D	2.21	0.41
1:C:105:THR:HG23	1:C:108:GLU:OE1	2.20	0.41
1:C:7:LYS:NZ	1:C:7:LYS:O	2.44	0.41
1:D:139:HIS:ND1	1:D:146:LEU:HD11	2.36	0.41
1:D:161:HIS:NE2	1:D:165:LYS:NZ	2.53	0.41
1:G:154:GLU:OE1	1:G:156:THR:HG22	2.21	0.41
1:G:277:CYS:HB2	1:H:415:TYR:HD2	1.86	0.41
1:H:171:ILE:O	1:H:173:LYS:HG2	2.21	0.41
1:G:412:GLN:HG2	1:H:277:CYS:SG	2.61	0.41
1:B:136:ASN:O	1:B:140:THR:HG23	2.20	0.40
1:B:153:SER:HB2	1:B:368:GLN:HE21	1.87	0.40
1:B:197:SER:OG	1:B:352:HIS:HD2	2.03	0.40
1:B:364:GLN:HE21	1:B:364:GLN:HA	1.86	0.40
1:D:160:VAL:HG11	1:D:178:ASN:ND2	2.36	0.40
1:D:208:VAL:HG22	1:D:209:MET:N	2.35	0.40
1:D:37:MET:HE2	1:D:38:TYR:CZ	2.56	0.40
1:E:178:ASN:ND2	1:E:181:ASP:HB2	2.36	0.40
1:E:153:SER:HB2	1:E:368:GLN:HE21	1.86	0.40
1:A:240:ILE:O	1:A:258:VAL:HA	2.21	0.40
1:A:364:GLN:HE21	1:A:364:GLN:CA	2.34	0.40
1:A:419:PRO:HB2	1:A:422:GLY:N	2.34	0.40
1:B:156:THR:CG2	1:B:159:GLY:N	2.75	0.40
1:B:295:VAL:HG12	1:B:305:ILE:HD13	2.03	0.40
1:C:160:VAL:HG11	1:C:178:ASN:ND2	2.36	0.40
1:C:300:HIS:H	2:C:432:NAD:C1D	2.21	0.40
1:G:246:ILE:O	1:G:250:GLN:HG3	2.21	0.40
1:H:364:GLN:CA	1:H:364:GLN:HE21	2.33	0.40
1:A:323:GLN:HG3	1:A:339:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:HA3	2:A:432:NAD:O5B	2.21	0.40
1:B:105:THR:C	1:B:107:GLU:N	2.75	0.40
1:B:183:VAL:HG11	1:B:431:TYR:CD1	2.57	0.40
1:B:57:VAL:HG23	1:B:84:GLN:HE21	1.87	0.40
1:C:10:ASP:HB3	1:C:13:LEU:HD22	2.03	0.40
1:C:360:SER:O	1:C:363:ASN:HB2	2.20	0.40
1:C:375:PRO:HB2	4:C:457:HOH:O	2.21	0.40
1:C:91:ILE:HA	1:C:91:ILE:HD13	1.85	0.40
1:D:74:ARG:HE	1:D:120:LYS:HZ3	1.67	0.40
1:E:91:ILE:HA	1:E:91:ILE:HD13	1.89	0.40
1:F:321:LYS:HB2	1:F:322:PRO:CD	2.52	0.40
1:G:9:ALA:HB2	1:G:101:TRP:HB2	2.02	0.40
1:H:385:LEU:HA	1:H:385:LEU:HD12	1.90	0.40
1:A:124:LEU:N	1:A:124:LEU:HD23	2.36	0.40
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.96	0.40
1:C:152:ILE:CG2	1:C:153:SER:N	2.84	0.40
1:C:3:LYS:HE2	1:C:115:GLN:NE2	2.34	0.40
1:C:57:VAL:O	1:C:60:ALA:HB3	2.21	0.40
1:D:300:HIS:H	2:D:432:NAD:C1D	2.19	0.40
1:D:409:THR:H	1:D:412:GLN:NE2	2.08	0.40
1:D:44:LEU:HB3	1:D:71:ALA:HB2	2.03	0.40
1:E:156:THR:CG2	1:E:159:GLY:N	2.74	0.40
1:E:172:LEU:HD22	1:E:174:VAL:H	1.86	0.40
1:E:307:VAL:H	1:E:308:LYS:NZ	2.20	0.40
1:E:9:ALA:HB2	1:E:101:TRP:HB2	2.03	0.40
1:F:134:LEU:O	1:F:138:ILE:HG12	2.22	0.40
1:G:180:ASN:O	1:G:186:SER:HB2	2.21	0.40
1:H:240:ILE:O	1:H:258:VAL:HA	2.21	0.40
1:A:124:LEU:O	1:A:124:LEU:HG	2.22	0.40
1:A:258:VAL:HB	1:B:403:VAL:HG13	2.01	0.40
1:B:35:ARG:NH2	1:B:64:GLU:HB2	2.36	0.40
1:C:6:TYR:OH	1:C:11:ILE:HD13	2.22	0.40
1:C:364:GLN:HE21	1:C:364:GLN:CA	2.33	0.40
1:D:153:SER:HB2	1:D:368:GLN:NE2	2.36	0.40
1:E:3:LYS:HE2	1:E:115:GLN:NE2	2.33	0.40
1:F:27:GLU:O	1:F:29:PRO:HD3	2.22	0.40
1:H:167:MET:HG2	1:H:172:LEU:HD12	2.03	0.40
1:H:59:THR:O	1:H:59:THR:HG22	2.21	0.40
1:H:45:LYS:HA	1:H:70:GLY:O	2.22	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	428/431 (99%)	409 (96%)	17 (4%)	2 (0%)	29	61
1	B	428/431 (99%)	408 (95%)	18 (4%)	2 (0%)	29	61
1	C	428/431 (99%)	409 (96%)	17 (4%)	2 (0%)	29	61
1	D	428/431 (99%)	408 (95%)	18 (4%)	2 (0%)	29	61
1	E	428/431 (99%)	409 (96%)	17 (4%)	2 (0%)	29	61
1	F	428/431 (99%)	410 (96%)	16 (4%)	2 (0%)	29	61
1	G	428/431 (99%)	410 (96%)	16 (4%)	2 (0%)	29	61
1	H	428/431 (99%)	408 (95%)	18 (4%)	2 (0%)	29	61
All	All	3424/3448 (99%)	3271 (96%)	137 (4%)	16 (0%)	29	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	GLY
1	B	422	GLY
1	C	422	GLY
1	D	422	GLY
1	E	422	GLY
1	F	422	GLY
1	G	422	GLY
1	H	422	GLY
1	H	300	HIS
1	A	300	HIS
1	D	300	HIS
1	E	300	HIS
1	F	300	HIS
1	G	300	HIS
1	B	300	HIS
1	C	300	HIS

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	353/353 (100%)	307 (87%)	46 (13%)	4	13
1	B	353/353 (100%)	309 (88%)	44 (12%)	4	14
1	C	353/353 (100%)	305 (86%)	48 (14%)	3	11
1	D	353/353 (100%)	306 (87%)	47 (13%)	4	12
1	E	353/353 (100%)	303 (86%)	50 (14%)	3	10
1	F	353/353 (100%)	307 (87%)	46 (13%)	4	13
1	G	353/353 (100%)	305 (86%)	48 (14%)	3	11
1	H	353/353 (100%)	302 (86%)	51 (14%)	3	10
All	All	2824/2824 (100%)	2444 (86%)	380 (14%)	4	11

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	7	LYS
1	A	11	ILE
1	A	13	LEU
1	A	26	ASN
1	A	41	SER
1	A	45	LYS
1	A	73	VAL
1	A	84	GLN
1	A	86	HIS
1	A	93	LYS
1	A	108	GLU
1	A	110	LEU
1	A	120	LYS
1	A	121	ASP
1	A	134	LEU
1	A	135	THR
1	A	144	GLN
1	A	146	LEU

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Mol	Chain	Res	Type
1	A	156	THR
1	A	161	HIS
1	A	167	MET
1	A	172	LEU
1	A	174	VAL
1	A	196	GLU
1	A	209	MET
1	A	232	ARG
1	A	241	THR
1	A	259	THR
1	A	277	CYS
1	A	282	LEU
1	A	288	GLN
1	A	308	LYS
1	A	334	ARG
1	A	337	LEU
1	A	342	ARG
1	A	364	GLN
1	A	371	LEU
1	A	382	VAL
1	A	385	LEU
1	A	388	LYS
1	A	398	LEU
1	A	402	ASN
1	A	408	LEU
1	A	410	GLU
1	A	418	MET
1	B	4	LEU
1	B	7	LYS
1	B	11	ILE
1	B	13	LEU
1	B	26	ASN
1	B	41	SER
1	B	45	LYS
1	B	73	VAL
1	B	84	GLN
1	B	86	HIS
1	B	93	LYS
1	B	108	GLU
1	B	110	LEU
1	B	120	LYS
1	B	121	ASP

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Mol	Chain	Res	Type
1	B	134	LEU
1	B	135	THR
1	B	144	GLN
1	B	147	SER
1	B	156	THR
1	B	161	HIS
1	B	167	MET
1	B	172	LEU
1	B	174	VAL
1	B	196	GLU
1	B	209	MET
1	B	241	THR
1	B	259	THR
1	B	277	CYS
1	B	282	LEU
1	B	288	GLN
1	B	308	LYS
1	B	337	LEU
1	B	342	ARG
1	B	364	GLN
1	B	371	LEU
1	B	382	VAL
1	B	385	LEU
1	B	388	LYS
1	B	398	LEU
1	B	402	ASN
1	B	408	LEU
1	B	410	GLU
1	B	418	MET
1	C	4	LEU
1	C	7	LYS
1	C	11	ILE
1	C	13	LEU
1	C	26	ASN
1	C	33	ARG
1	C	41	SER
1	C	45	LYS
1	C	73	VAL
1	C	84	GLN
1	C	86	HIS
1	C	93	LYS
1	C	108	GLU

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Mol	Chain	Res	Type
1	C	110	LEU
1	C	120	LYS
1	C	121	ASP
1	C	134	LEU
1	C	135	THR
1	C	144	GLN
1	C	146	LEU
1	C	147	SER
1	C	156	THR
1	C	161	HIS
1	C	167	MET
1	C	172	LEU
1	C	174	VAL
1	C	196	GLU
1	C	209	MET
1	C	241	THR
1	C	259	THR
1	C	266	LYS
1	C	277	CYS
1	C	282	LEU
1	C	288	GLN
1	C	308	LYS
1	C	337	LEU
1	C	342	ARG
1	C	364	GLN
1	C	371	LEU
1	C	382	VAL
1	C	385	LEU
1	C	388	LYS
1	C	398	LEU
1	C	402	ASN
1	C	408	LEU
1	C	410	GLU
1	C	418	MET
1	C	423	PRO
1	D	2	ASP
1	D	4	LEU
1	D	7	LYS
1	D	11	ILE
1	D	13	LEU
1	D	26	ASN
1	D	33	ARG

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Mol	Chain	Res	Type
1	D	41	SER
1	D	45	LYS
1	D	73	VAL
1	D	84	GLN
1	D	86	HIS
1	D	93	LYS
1	D	108	GLU
1	D	110	LEU
1	D	120	LYS
1	D	121	ASP
1	D	134	LEU
1	D	135	THR
1	D	144	GLN
1	D	147	SER
1	D	156	THR
1	D	161	HIS
1	D	167	MET
1	D	172	LEU
1	D	174	VAL
1	D	196	GLU
1	D	209	MET
1	D	241	THR
1	D	259	THR
1	D	277	CYS
1	D	282	LEU
1	D	288	GLN
1	D	308	LYS
1	D	334	ARG
1	D	337	LEU
1	D	342	ARG
1	D	364	GLN
1	D	371	LEU
1	D	382	VAL
1	D	385	LEU
1	D	388	LYS
1	D	398	LEU
1	D	402	ASN
1	D	408	LEU
1	D	410	GLU
1	D	418	MET
1	E	2	ASP
1	E	4	LEU

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Mol	Chain	Res	Type
1	E	7	LYS
1	E	11	ILE
1	E	13	LEU
1	E	26	ASN
1	E	33	ARG
1	E	41	SER
1	E	45	LYS
1	E	73	VAL
1	E	84	GLN
1	E	86	HIS
1	E	93	LYS
1	E	108	GLU
1	E	110	LEU
1	E	120	LYS
1	E	121	ASP
1	E	134	LEU
1	E	135	THR
1	E	144	GLN
1	E	146	LEU
1	E	147	SER
1	E	156	THR
1	E	161	HIS
1	E	167	MET
1	E	172	LEU
1	E	174	VAL
1	E	196	GLU
1	E	209	MET
1	E	241	THR
1	E	242	GLU
1	E	259	THR
1	E	277	CYS
1	E	282	LEU
1	E	288	GLN
1	E	302	ASP
1	E	308	LYS
1	E	334	ARG
1	E	337	LEU
1	E	342	ARG
1	E	364	GLN
1	E	371	LEU
1	E	382	VAL
1	E	385	LEU

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Mol	Chain	Res	Type
1	E	388	LYS
1	E	398	LEU
1	E	402	ASN
1	E	408	LEU
1	E	410	GLU
1	E	418	MET
1	F	4	LEU
1	F	7	LYS
1	F	11	ILE
1	F	13	LEU
1	F	26	ASN
1	F	41	SER
1	F	45	LYS
1	F	73	VAL
1	F	84	GLN
1	F	86	HIS
1	F	93	LYS
1	F	108	GLU
1	F	110	LEU
1	F	120	LYS
1	F	121	ASP
1	F	134	LEU
1	F	135	THR
1	F	144	GLN
1	F	146	LEU
1	F	156	THR
1	F	161	HIS
1	F	167	MET
1	F	172	LEU
1	F	174	VAL
1	F	196	GLU
1	F	209	MET
1	F	241	THR
1	F	259	THR
1	F	277	CYS
1	F	282	LEU
1	F	288	GLN
1	F	302	ASP
1	F	308	LYS
1	F	337	LEU
1	F	342	ARG
1	F	364	GLN

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Mol	Chain	Res	Type
1	F	371	LEU
1	F	382	VAL
1	F	385	LEU
1	F	388	LYS
1	F	398	LEU
1	F	402	ASN
1	F	408	LEU
1	F	410	GLU
1	F	418	MET
1	F	423	PRO
1	G	2	ASP
1	G	4	LEU
1	G	7	LYS
1	G	11	ILE
1	G	13	LEU
1	G	26	ASN
1	G	33	ARG
1	G	41	SER
1	G	45	LYS
1	G	73	VAL
1	G	74	ARG
1	G	84	GLN
1	G	86	HIS
1	G	93	LYS
1	G	108	GLU
1	G	110	LEU
1	G	120	LYS
1	G	121	ASP
1	G	134	LEU
1	G	135	THR
1	G	144	GLN
1	G	147	SER
1	G	156	THR
1	G	161	HIS
1	G	167	MET
1	G	172	LEU
1	G	174	VAL
1	G	196	GLU
1	G	209	MET
1	G	241	THR
1	G	242	GLU
1	G	259	THR

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Mol	Chain	Res	Type
1	G	277	CYS
1	G	282	LEU
1	G	288	GLN
1	G	308	LYS
1	G	337	LEU
1	G	342	ARG
1	G	364	GLN
1	G	371	LEU
1	G	382	VAL
1	G	385	LEU
1	G	388	LYS
1	G	398	LEU
1	G	402	ASN
1	G	408	LEU
1	G	410	GLU
1	G	418	MET
1	H	2	ASP
1	H	4	LEU
1	H	7	LYS
1	H	11	ILE
1	H	13	LEU
1	H	26	ASN
1	H	33	ARG
1	H	41	SER
1	H	45	LYS
1	H	73	VAL
1	H	84	GLN
1	H	86	HIS
1	H	93	LYS
1	H	108	GLU
1	H	110	LEU
1	H	120	LYS
1	H	121	ASP
1	H	134	LEU
1	H	135	THR
1	H	144	GLN
1	H	146	LEU
1	H	147	SER
1	H	156	THR
1	H	161	HIS
1	H	167	MET
1	H	172	LEU

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Mol	Chain	Res	Type
1	H	174	VAL
1	H	196	GLU
1	H	209	MET
1	H	241	THR
1	H	259	THR
1	H	266	LYS
1	H	277	CYS
1	H	282	LEU
1	H	288	GLN
1	H	302	ASP
1	H	308	LYS
1	H	334	ARG
1	H	337	LEU
1	H	342	ARG
1	H	364	GLN
1	H	371	LEU
1	H	382	VAL
1	H	385	LEU
1	H	388	LYS
1	H	398	LEU
1	H	402	ASN
1	H	408	LEU
1	H	410	GLU
1	H	418	MET
1	H	423	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	84	GLN
1	A	136	ASN
1	A	162	ASN
1	A	247	ASN
1	A	250	GLN
1	A	352	HIS
1	A	364	GLN
1	A	368	GLN
1	A	383	HIS
1	A	412	GLN
1	A	414	GLN
1	B	26	ASN

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Mol	Chain	Res	Type
1	B	84	GLN
1	B	115	GLN
1	B	136	ASN
1	B	162	ASN
1	B	247	ASN
1	B	250	GLN
1	B	288	GLN
1	B	352	HIS
1	B	364	GLN
1	B	368	GLN
1	B	383	HIS
1	B	412	GLN
1	B	414	GLN
1	C	26	ASN
1	C	84	GLN
1	C	247	ASN
1	C	250	GLN
1	C	288	GLN
1	C	352	HIS
1	C	364	GLN
1	C	368	GLN
1	C	383	HIS
1	C	412	GLN
1	C	414	GLN
1	D	26	ASN
1	D	84	GLN
1	D	136	ASN
1	D	162	ASN
1	D	247	ASN
1	D	250	GLN
1	D	352	HIS
1	D	364	GLN
1	D	368	GLN
1	D	383	HIS
1	D	412	GLN
1	D	414	GLN
1	E	26	ASN
1	E	84	GLN
1	E	136	ASN
1	E	162	ASN
1	E	247	ASN
1	E	250	GLN

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Mol	Chain	Res	Type
1	E	352	HIS
1	E	364	GLN
1	E	368	GLN
1	E	383	HIS
1	E	412	GLN
1	E	414	GLN
1	F	26	ASN
1	F	84	GLN
1	F	136	ASN
1	F	162	ASN
1	F	247	ASN
1	F	250	GLN
1	F	352	HIS
1	F	364	GLN
1	F	368	GLN
1	F	383	HIS
1	F	412	GLN
1	F	414	GLN
1	G	26	ASN
1	G	84	GLN
1	G	136	ASN
1	G	162	ASN
1	G	247	ASN
1	G	250	GLN
1	G	288	GLN
1	G	352	HIS
1	G	364	GLN
1	G	368	GLN
1	G	383	HIS
1	G	412	GLN
1	G	414	GLN
1	H	26	ASN
1	H	84	GLN
1	H	136	ASN
1	H	162	ASN
1	H	247	ASN
1	H	250	GLN
1	H	352	HIS
1	H	364	GLN
1	H	368	GLN
1	H	383	HIS
1	H	412	GLN

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Mol	Chain	Res	Type
1	H	414	GLN

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

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	3DD	E	433	-	15,19,19	2.16	4 (26%)	14,27,27	1.92	4 (28%)
3	3DD	G	433	-	15,19,19	2.14	4 (26%)	14,27,27	1.90	4 (28%)
3	3DD	H	433	-	15,19,19	2.21	7 (46%)	14,27,27	1.93	4 (28%)
3	3DD	A	433	-	15,19,19	2.12	5 (33%)	14,27,27	1.90	4 (28%)
3	3DD	C	433	-	15,19,19	2.06	4 (26%)	14,27,27	1.98	4 (28%)
2	NAD	C	432	-	42,48,48	2.25	8 (19%)	50,73,73	1.75	9 (18%)
2	NAD	F	432	-	42,48,48	2.10	10 (23%)	50,73,73	1.77	9 (18%)
2	NAD	A	432	-	42,48,48	2.29	8 (19%)	50,73,73	1.73	9 (18%)
2	NAD	D	432	-	42,48,48	2.21	8 (19%)	50,73,73	1.83	9 (18%)
2	NAD	G	432	-	42,48,48	2.13	9 (21%)	50,73,73	1.75	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	E	432	-	42,48,48	2.18	10 (23%)	50,73,73	1.75	9 (18%)
3	3DD	D	433	-	15,19,19	1.91	5 (33%)	14,27,27	1.88	4 (28%)
3	3DD	F	433	-	15,19,19	2.12	5 (33%)	14,27,27	1.92	4 (28%)
2	NAD	B	432	-	42,48,48	2.10	8 (19%)	50,73,73	1.78	8 (16%)
3	3DD	B	433	-	15,19,19	2.04	5 (33%)	14,27,27	1.92	4 (28%)
2	NAD	H	432	-	42,48,48	2.27	8 (19%)	50,73,73	1.85	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3DD	E	433	-	-	0/6/12/12	0/2/2/2
3	3DD	G	433	-	-	0/6/12/12	0/2/2/2
3	3DD	H	433	-	-	0/6/12/12	0/2/2/2
3	3DD	A	433	-	-	0/6/12/12	0/2/2/2
3	3DD	C	433	-	-	0/6/12/12	0/2/2/2
2	NAD	C	432	-	-	5/26/62/62	0/5/5/5
2	NAD	F	432	-	-	5/26/62/62	0/5/5/5
2	NAD	A	432	-	-	5/26/62/62	0/5/5/5
2	NAD	D	432	-	-	5/26/62/62	0/5/5/5
2	NAD	G	432	-	-	5/26/62/62	0/5/5/5
2	NAD	E	432	-	-	5/26/62/62	0/5/5/5
3	3DD	D	433	-	-	0/6/12/12	0/2/2/2
3	3DD	F	433	-	-	0/6/12/12	0/2/2/2
2	NAD	B	432	-	-	5/26/62/62	0/5/5/5
3	3DD	B	433	-	-	0/6/12/12	0/2/2/2
2	NAD	H	432	-	-	5/26/62/62	0/5/5/5

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	432	NAD	C5N-C4N	6.89	1.53	1.38
2	H	432	NAD	C5N-C4N	6.79	1.53	1.38
2	C	432	NAD	C5N-C4N	6.78	1.53	1.38
2	B	432	NAD	C5N-C4N	6.54	1.52	1.38
2	D	432	NAD	C5N-C4N	6.53	1.52	1.38
2	E	432	NAD	C5N-C4N	6.46	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	432	NAD	C4N-C3N	6.36	1.50	1.39
2	G	432	NAD	C5N-C4N	6.30	1.52	1.38
2	D	432	NAD	C4N-C3N	6.29	1.50	1.39
2	A	432	NAD	C2N-N1N	6.26	1.42	1.35
2	C	432	NAD	C4N-C3N	6.23	1.50	1.39
2	F	432	NAD	C5N-C4N	6.21	1.52	1.38
2	A	432	NAD	C4N-C3N	6.11	1.49	1.39
2	H	432	NAD	C2N-N1N	6.08	1.42	1.35
2	C	432	NAD	C2N-N1N	5.99	1.42	1.35
2	G	432	NAD	C2N-N1N	5.85	1.42	1.35
2	B	432	NAD	C2N-N1N	5.80	1.42	1.35
2	H	432	NAD	C2N-C3N	5.71	1.47	1.39
2	C	432	NAD	C2N-C3N	5.71	1.47	1.39
2	D	432	NAD	C2N-C3N	5.67	1.47	1.39
2	F	432	NAD	C4N-C3N	5.63	1.48	1.39
2	E	432	NAD	C4N-C3N	5.62	1.48	1.39
2	A	432	NAD	C2N-C3N	5.62	1.47	1.39
2	E	432	NAD	C2N-N1N	5.60	1.41	1.35
2	D	432	NAD	C2N-N1N	5.56	1.41	1.35
2	G	432	NAD	C4N-C3N	5.52	1.48	1.39
2	B	432	NAD	C4N-C3N	5.41	1.48	1.39
2	E	432	NAD	C2N-C3N	5.20	1.47	1.39
2	F	432	NAD	C2N-N1N	4.93	1.41	1.35
2	G	432	NAD	C2N-C3N	4.83	1.46	1.39
2	F	432	NAD	C2N-C3N	4.81	1.46	1.39
3	E	433	3DD	C2'-C3'	4.65	1.57	1.53
2	B	432	NAD	C2N-C3N	4.65	1.46	1.39
3	B	433	3DD	C8-N7	-4.40	1.26	1.34
2	D	432	NAD	C6N-N1N	4.40	1.46	1.35
2	E	432	NAD	O4B-C1B	-4.31	1.35	1.41
3	C	433	3DD	C2'-C3'	4.26	1.57	1.53
3	G	433	3DD	C2'-C3'	4.21	1.57	1.53
3	F	433	3DD	C2'-C3'	4.18	1.57	1.53
2	A	432	NAD	O4B-C1B	-4.13	1.35	1.41
2	H	432	NAD	C6N-N1N	4.08	1.45	1.35
2	H	432	NAD	O4B-C1B	-4.03	1.35	1.41
2	G	432	NAD	O4B-C1B	-3.97	1.35	1.41
2	B	432	NAD	C6N-N1N	3.96	1.45	1.35
3	F	433	3DD	C8-N7	-3.95	1.27	1.34
3	A	433	3DD	C8-N7	-3.92	1.27	1.34
2	E	432	NAD	C6N-N1N	3.91	1.45	1.35
2	A	432	NAD	C6N-N1N	3.90	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	433	3DD	C8-N7	-3.89	1.27	1.34
2	G	432	NAD	C6N-N1N	3.83	1.44	1.35
3	G	433	3DD	C8-N7	-3.82	1.27	1.34
2	C	432	NAD	O4B-C1B	-3.78	1.35	1.41
2	C	432	NAD	C6N-N1N	3.76	1.44	1.35
3	G	433	3DD	C4-C5	3.73	1.48	1.40
3	E	433	3DD	C8-N7	-3.72	1.28	1.34
2	B	432	NAD	O4B-C1B	-3.72	1.35	1.41
3	A	433	3DD	C2'-C3'	3.71	1.57	1.53
3	B	433	3DD	C2'-C3'	3.69	1.57	1.53
3	H	433	3DD	C2'-C3'	3.67	1.57	1.53
2	F	432	NAD	O4B-C1B	-3.66	1.36	1.41
3	H	433	3DD	C4-C5	3.66	1.48	1.40
2	F	432	NAD	C6N-N1N	3.64	1.44	1.35
2	D	432	NAD	O4B-C1B	-3.51	1.36	1.41
3	H	433	3DD	C8-N7	-3.51	1.28	1.34
3	D	433	3DD	C4-C5	3.41	1.47	1.40
3	E	433	3DD	C4-C5	3.41	1.47	1.40
3	D	433	3DD	C8-N7	-3.31	1.28	1.34
3	C	433	3DD	C4-C5	3.29	1.47	1.40
3	D	433	3DD	C2'-C3'	3.23	1.56	1.53
3	A	433	3DD	C4-C5	3.14	1.46	1.40
2	F	432	NAD	C2A-N1A	2.90	1.39	1.33
3	F	433	3DD	C4-C5	2.89	1.46	1.40
3	H	433	3DD	C4-N9	-2.85	1.35	1.39
3	A	433	3DD	C4-N9	-2.84	1.35	1.39
3	F	433	3DD	C4-N9	-2.81	1.35	1.39
2	A	432	NAD	C2A-N1A	2.70	1.38	1.33
2	F	432	NAD	C7N-N7N	2.61	1.38	1.33
3	C	433	3DD	C2-N1	2.60	1.40	1.34
3	B	433	3DD	C4-C5	2.59	1.45	1.40
2	G	432	NAD	C6N-C5N	-2.56	1.32	1.38
2	F	432	NAD	C2D-C1D	-2.54	1.49	1.53
2	E	432	NAD	C7N-N7N	2.53	1.37	1.33
2	F	432	NAD	C6N-C5N	-2.48	1.33	1.38
2	B	432	NAD	C2A-N1A	2.46	1.38	1.33
3	A	433	3DD	C3-C4	-2.45	1.36	1.41
2	D	432	NAD	C2A-N1A	2.44	1.38	1.33
2	E	432	NAD	C6N-C5N	-2.40	1.33	1.38
3	H	433	3DD	C3-C4	-2.37	1.36	1.41
2	G	432	NAD	C7N-N7N	2.35	1.37	1.33
3	H	433	3DD	C1'-N9	-2.35	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	433	3DD	C2-N1	2.34	1.39	1.34
2	E	432	NAD	C2A-N1A	2.33	1.38	1.33
3	H	433	3DD	C2-N1	2.30	1.39	1.34
2	E	432	NAD	C2D-C1D	-2.24	1.50	1.53
2	G	432	NAD	C2A-N1A	2.21	1.38	1.33
2	C	432	NAD	C7N-N7N	2.20	1.37	1.33
3	B	433	3DD	C4-N9	-2.17	1.36	1.39
2	H	432	NAD	C2D-C1D	-2.17	1.50	1.53
3	F	433	3DD	C3-C4	-2.17	1.36	1.41
2	C	432	NAD	C2D-C1D	-2.15	1.50	1.53
2	D	432	NAD	C6N-C5N	-2.14	1.33	1.38
2	H	432	NAD	C2A-N1A	2.11	1.37	1.33
3	D	433	3DD	C5-N7	-2.10	1.32	1.39
3	B	433	3DD	C3-C4	-2.09	1.36	1.41
3	D	433	3DD	C4-N9	-2.07	1.36	1.39
2	B	432	NAD	C6N-C5N	-2.06	1.34	1.38
3	E	433	3DD	C3-C4	-2.05	1.37	1.41
2	A	432	NAD	C6N-C5N	-2.04	1.34	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	432	NAD	C3N-C7N-N7N	6.54	125.60	117.75
2	H	432	NAD	C3N-C7N-N7N	6.52	125.58	117.75
2	H	432	NAD	O7N-C7N-C3N	-6.03	112.42	119.63
2	F	432	NAD	C3N-C7N-N7N	6.01	124.97	117.75
2	C	432	NAD	C3N-C7N-N7N	5.98	124.93	117.75
2	B	432	NAD	C3N-C7N-N7N	5.94	124.87	117.75
2	A	432	NAD	C3N-C7N-N7N	5.85	124.77	117.75
2	G	432	NAD	C3N-C7N-N7N	5.82	124.73	117.75
2	F	432	NAD	O7N-C7N-C3N	-5.78	112.71	119.63
2	E	432	NAD	C3N-C7N-N7N	5.76	124.66	117.75
2	D	432	NAD	O7N-C7N-C3N	-5.60	112.93	119.63
2	G	432	NAD	O7N-C7N-C3N	-5.58	112.95	119.63
2	B	432	NAD	O7N-C7N-C3N	-5.52	113.03	119.63
2	E	432	NAD	O7N-C7N-C3N	-5.50	113.06	119.63
2	C	432	NAD	O7N-C7N-C3N	-5.23	113.38	119.63
2	A	432	NAD	O7N-C7N-C3N	-5.00	113.64	119.63
2	B	432	NAD	O4B-C1B-C2B	-4.57	100.25	106.93
2	D	432	NAD	O4B-C1B-C2B	-4.40	100.50	106.93
2	D	432	NAD	C6N-N1N-C2N	-4.37	117.99	121.97
3	E	433	3DD	C1'-N9-C4	4.37	131.63	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	432	NAD	C6N-N1N-C2N	-4.35	118.01	121.97
3	B	433	3DD	C1'-N9-C4	4.34	131.59	125.43
2	F	432	NAD	C6N-N1N-C2N	-4.33	118.03	121.97
2	A	432	NAD	O4B-C1B-C2B	-4.31	100.62	106.93
3	C	433	3DD	C1'-N9-C4	4.27	131.49	125.43
2	H	432	NAD	C6N-N1N-C2N	-4.26	118.09	121.97
3	F	433	3DD	C1'-N9-C4	4.26	131.48	125.43
3	H	433	3DD	C1'-N9-C4	4.26	131.47	125.43
3	D	433	3DD	C1'-N9-C4	4.24	131.45	125.43
3	A	433	3DD	C1'-N9-C4	4.24	131.44	125.43
2	E	432	NAD	O4B-C1B-C2B	-4.21	100.78	106.93
3	G	433	3DD	C1'-N9-C4	4.20	131.40	125.43
2	E	432	NAD	C6N-N1N-C2N	-4.20	118.14	121.97
2	G	432	NAD	C6N-N1N-C2N	-4.15	118.19	121.97
2	A	432	NAD	C6N-N1N-C2N	-4.14	118.20	121.97
2	C	432	NAD	C6N-N1N-C2N	-4.13	118.21	121.97
2	H	432	NAD	O4B-C1B-C2B	-4.12	100.91	106.93
2	G	432	NAD	O4B-C1B-C2B	-4.11	100.92	106.93
2	F	432	NAD	O4B-C1B-C2B	-3.94	101.17	106.93
2	C	432	NAD	O4B-C1B-C2B	-3.87	101.27	106.93
3	C	433	3DD	C2-N1-C6	3.73	123.07	117.61
3	G	433	3DD	C2-N1-C6	3.49	122.72	117.61
2	C	432	NAD	C5N-C4N-C3N	-3.44	116.28	120.34
3	H	433	3DD	C2-N1-C6	3.43	122.63	117.61
3	A	433	3DD	O3'-C3'-C2'	3.42	118.15	109.63
3	E	433	3DD	C2-N1-C6	3.41	122.61	117.61
3	B	433	3DD	C2-N1-C6	3.39	122.58	117.61
2	A	432	NAD	C5N-C4N-C3N	-3.38	116.34	120.34
2	H	432	NAD	C5N-C4N-C3N	-3.37	116.36	120.34
3	F	433	3DD	C2-N1-C6	3.37	122.54	117.61
3	H	433	3DD	O3'-C3'-C2'	3.37	118.03	109.63
3	G	433	3DD	O3'-C3'-C2'	3.27	117.80	109.63
3	D	433	3DD	C2-N1-C6	3.27	122.40	117.61
3	D	433	3DD	O3'-C3'-C2'	3.26	117.75	109.63
3	A	433	3DD	C2-N1-C6	3.23	122.34	117.61
3	B	433	3DD	O3'-C3'-C2'	3.22	117.67	109.63
3	E	433	3DD	O3'-C3'-C2'	3.20	117.61	109.63
2	E	432	NAD	C5N-C4N-C3N	-3.19	116.57	120.34
2	F	432	NAD	C5N-C4N-C3N	-3.18	116.58	120.34
3	C	433	3DD	O3'-C3'-C2'	3.18	117.57	109.63
2	D	432	NAD	C5N-C4N-C3N	-3.18	116.58	120.34
2	B	432	NAD	C5N-C4N-C3N	-3.13	116.64	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	432	NAD	C5N-C4N-C3N	-3.02	116.77	120.34
3	F	433	3DD	O3'-C3'-C2'	2.99	117.10	109.63
2	F	432	NAD	C5N-C6N-N1N	2.96	124.64	120.40
2	D	432	NAD	C5N-C6N-N1N	2.93	124.61	120.40
2	H	432	NAD	C5N-C6N-N1N	2.83	124.46	120.40
2	C	432	NAD	C5N-C6N-N1N	2.79	124.40	120.40
2	C	432	NAD	C4A-C5A-N7A	2.77	112.29	109.40
2	A	432	NAD	C5N-C6N-N1N	2.70	124.27	120.40
2	B	432	NAD	C5N-C6N-N1N	2.69	124.26	120.40
2	E	432	NAD	C5N-C6N-N1N	2.68	124.25	120.40
2	E	432	NAD	C5A-C6A-N6A	2.67	124.41	120.35
2	G	432	NAD	C5N-C6N-N1N	2.67	124.23	120.40
3	C	433	3DD	C3-C2-N1	-2.65	121.20	123.81
2	A	432	NAD	C5A-C6A-N6A	2.58	124.27	120.35
2	G	432	NAD	C4A-C5A-N7A	2.56	112.07	109.40
3	F	433	3DD	C3-C2-N1	-2.51	121.34	123.81
2	F	432	NAD	C4A-C5A-N7A	2.42	111.92	109.40
2	B	432	NAD	C4A-C5A-N7A	2.41	111.91	109.40
2	G	432	NAD	C5A-C6A-N6A	2.38	123.97	120.35
3	B	433	3DD	C3-C2-N1	-2.37	121.47	123.81
2	A	432	NAD	C4A-C5A-N7A	2.37	111.87	109.40
2	E	432	NAD	C4A-C5A-N7A	2.36	111.86	109.40
2	H	432	NAD	C4A-C5A-N7A	2.32	111.82	109.40
2	D	432	NAD	C5A-C6A-N6A	2.31	123.87	120.35
2	D	432	NAD	C4A-C5A-N7A	2.23	111.72	109.40
3	H	433	3DD	C3-C2-N1	-2.23	121.62	123.81
2	D	432	NAD	O5B-C5B-C4B	-2.21	101.38	108.99
2	C	432	NAD	C5A-C6A-N6A	2.21	123.70	120.35
2	F	432	NAD	C5A-C6A-N6A	2.20	123.70	120.35
2	H	432	NAD	C5A-C6A-N6A	2.20	123.69	120.35
2	F	432	NAD	O5B-C5B-C4B	-2.16	101.56	108.99
3	D	433	3DD	C3-C2-N1	-2.15	121.69	123.81
2	B	432	NAD	C5A-C6A-N6A	2.15	123.61	120.35
3	G	433	3DD	C3-C2-N1	-2.15	121.70	123.81
3	A	433	3DD	C3-C2-N1	-2.12	121.72	123.81
3	E	433	3DD	C3-C2-N1	-2.11	121.73	123.81
2	C	432	NAD	O5B-C5B-C4B	-2.09	101.80	108.99
2	A	432	NAD	O5B-C5B-C4B	-2.08	101.82	108.99
2	H	432	NAD	O5B-C5B-C4B	-2.05	101.92	108.99
2	E	432	NAD	O5B-C5B-C4B	-2.04	101.96	108.99

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	432	NAD	O4D-C1D-N1N-C2N
2	C	432	NAD	O4D-C1D-N1N-C6N
2	C	432	NAD	C2D-C1D-N1N-C2N
2	C	432	NAD	C2D-C1D-N1N-C6N
2	F	432	NAD	O4D-C1D-N1N-C2N
2	F	432	NAD	O4D-C1D-N1N-C6N
2	F	432	NAD	C2D-C1D-N1N-C2N
2	F	432	NAD	C2D-C1D-N1N-C6N
2	A	432	NAD	O4D-C1D-N1N-C2N
2	A	432	NAD	O4D-C1D-N1N-C6N
2	A	432	NAD	C2D-C1D-N1N-C2N
2	A	432	NAD	C2D-C1D-N1N-C6N
2	D	432	NAD	O4D-C1D-N1N-C2N
2	D	432	NAD	O4D-C1D-N1N-C6N
2	D	432	NAD	C2D-C1D-N1N-C2N
2	D	432	NAD	C2D-C1D-N1N-C6N
2	G	432	NAD	O4D-C1D-N1N-C2N
2	G	432	NAD	O4D-C1D-N1N-C6N
2	G	432	NAD	C2D-C1D-N1N-C2N
2	G	432	NAD	C2D-C1D-N1N-C6N
2	E	432	NAD	O4D-C1D-N1N-C2N
2	E	432	NAD	O4D-C1D-N1N-C6N
2	E	432	NAD	C2D-C1D-N1N-C2N
2	E	432	NAD	C2D-C1D-N1N-C6N
2	B	432	NAD	O4D-C1D-N1N-C2N
2	B	432	NAD	O4D-C1D-N1N-C6N
2	B	432	NAD	C2D-C1D-N1N-C2N
2	B	432	NAD	C2D-C1D-N1N-C6N
2	H	432	NAD	O4D-C1D-N1N-C2N
2	H	432	NAD	O4D-C1D-N1N-C6N
2	H	432	NAD	C2D-C1D-N1N-C2N
2	H	432	NAD	C2D-C1D-N1N-C6N
2	E	432	NAD	O4B-C4B-C5B-O5B
2	B	432	NAD	O4B-C4B-C5B-O5B
2	H	432	NAD	O4B-C4B-C5B-O5B
2	F	432	NAD	O4B-C4B-C5B-O5B
2	A	432	NAD	O4B-C4B-C5B-O5B
2	D	432	NAD	O4B-C4B-C5B-O5B
2	C	432	NAD	O4B-C4B-C5B-O5B
2	G	432	NAD	O4B-C4B-C5B-O5B

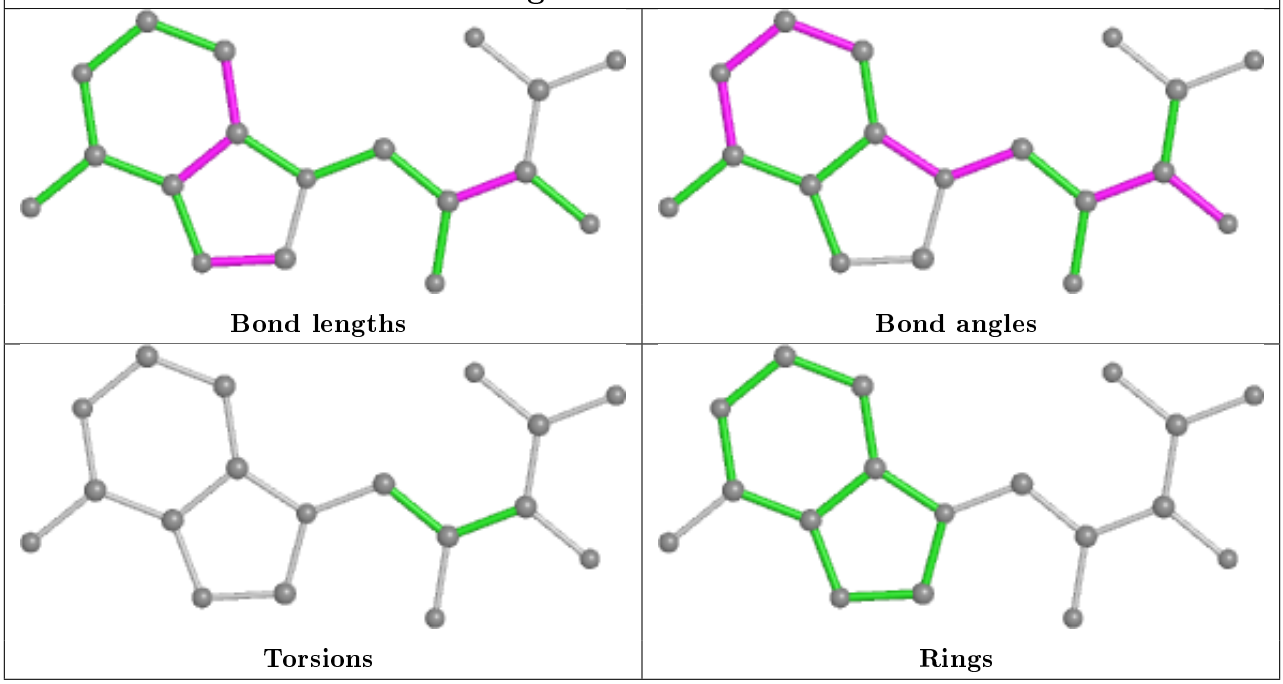
There are no ring outliers.

8 monomers are involved in 43 short contacts:

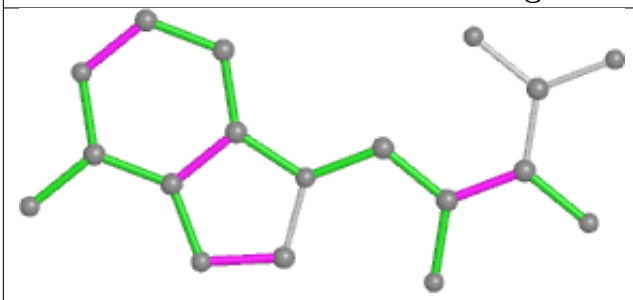
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	432	NAD	6	0
2	F	432	NAD	5	0
2	A	432	NAD	6	0
2	D	432	NAD	6	0
2	G	432	NAD	5	0
2	E	432	NAD	6	0
2	B	432	NAD	5	0
2	H	432	NAD	4	0

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.

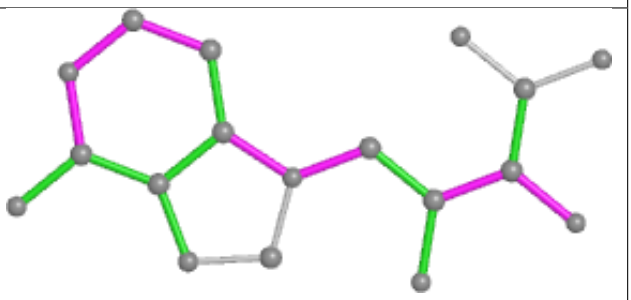
Ligand 3DD E 433



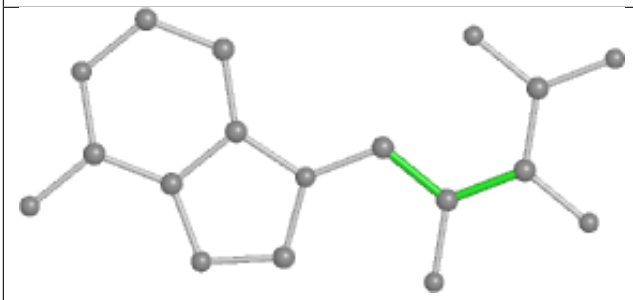
Ligand 3DD G 433



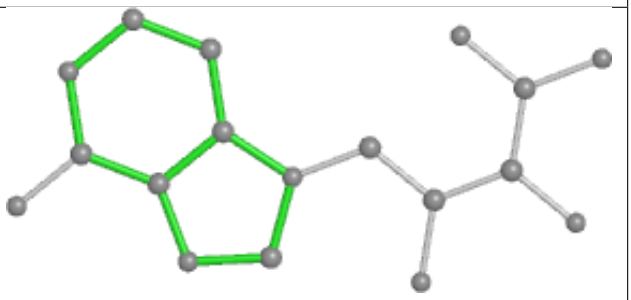
Bond lengths



Bond angles

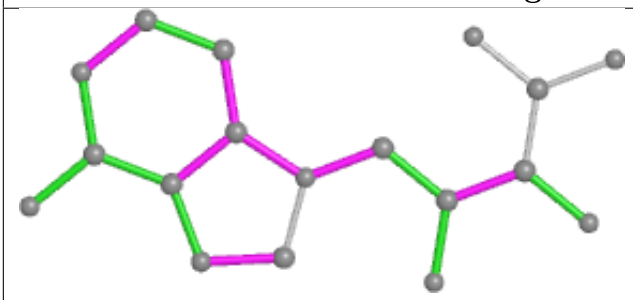


Torsions

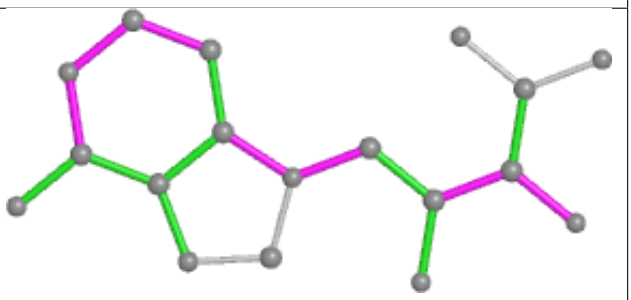


Rings

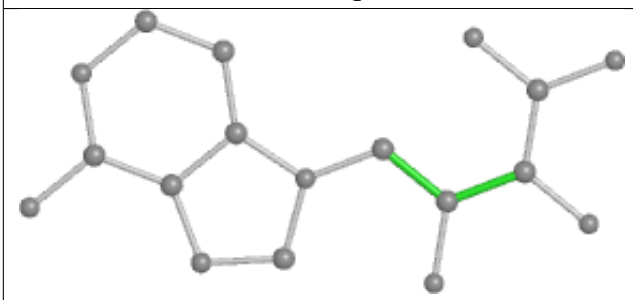
Ligand 3DD H 433



Bond lengths



Bond angles



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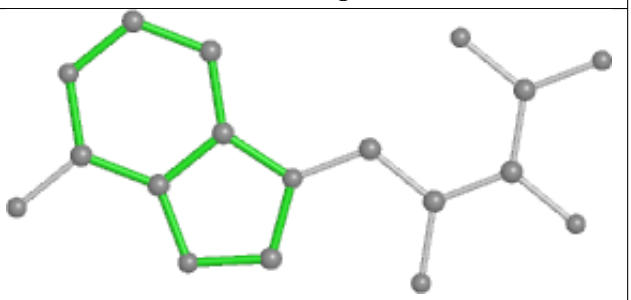
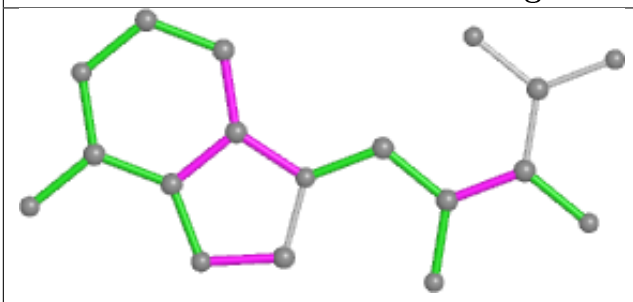
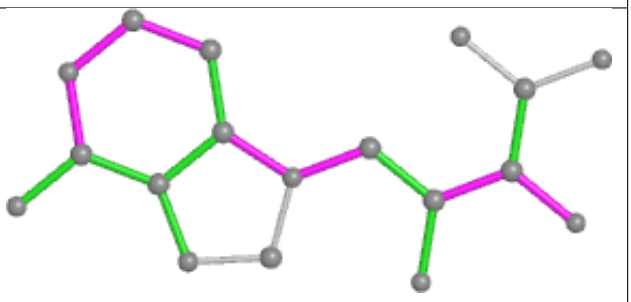


Rings

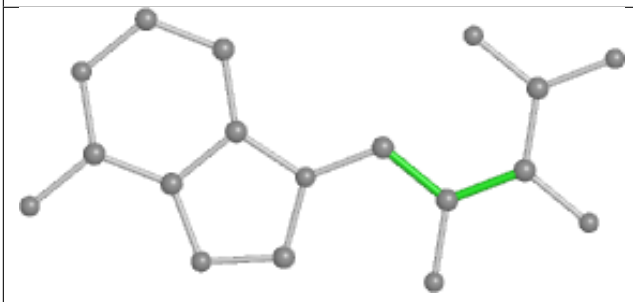
Ligand 3DD A 433



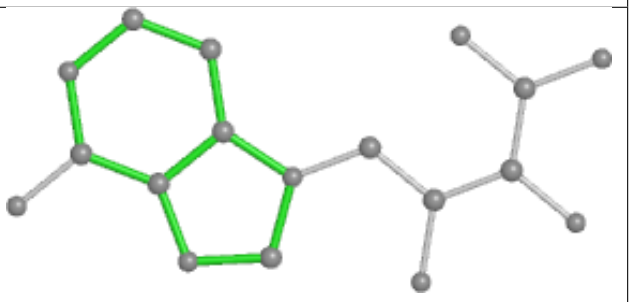
Bond lengths



Bond angles

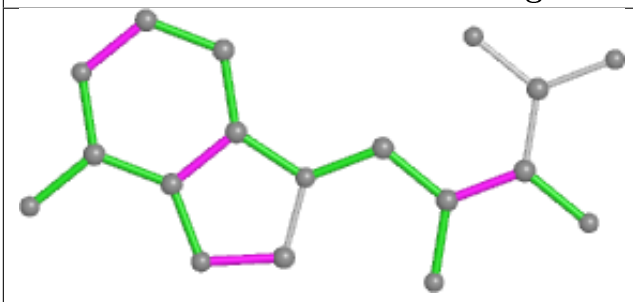


Torsions

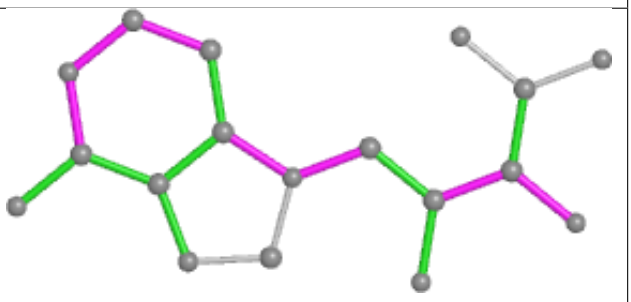


Rings

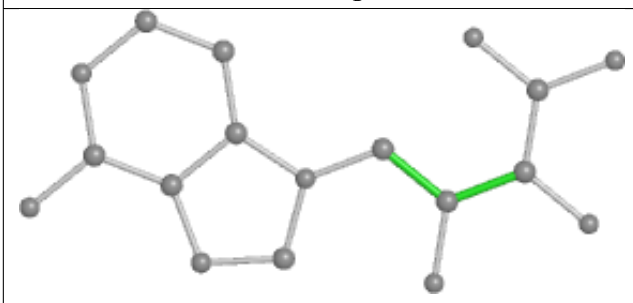
Ligand 3DD C 433



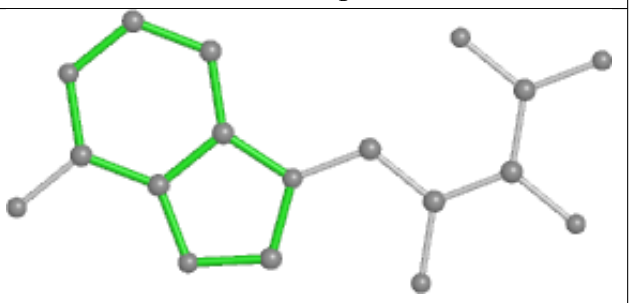
Bond lengths



Bond angles

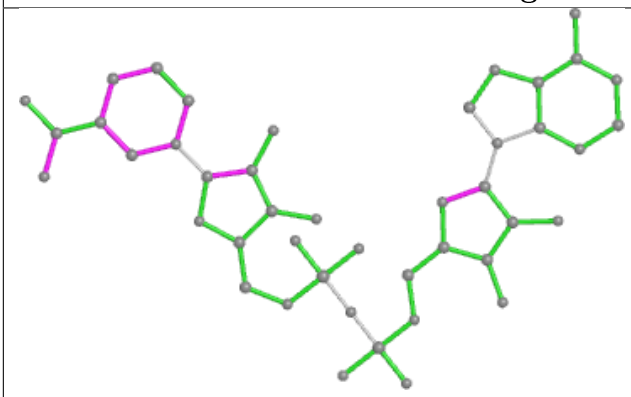


Torsions

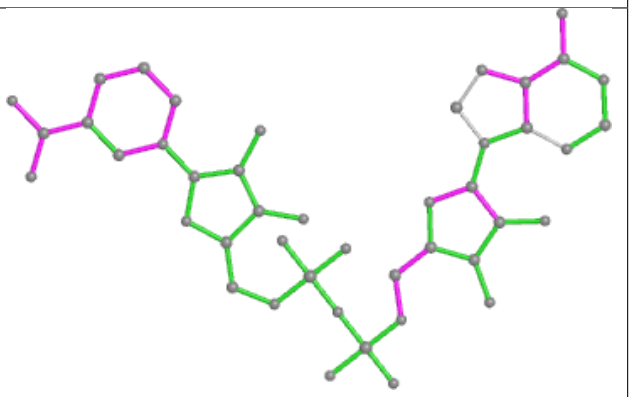


Rings

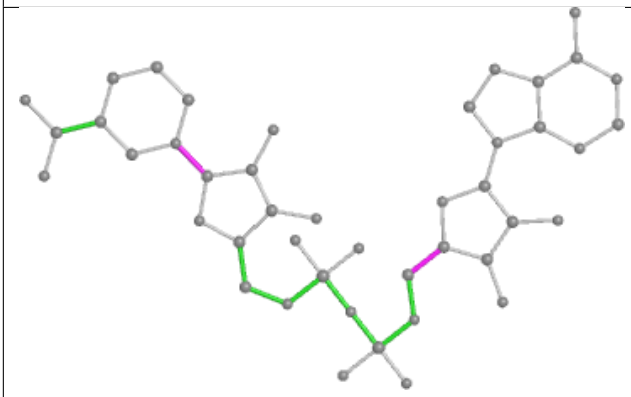
Ligand NAD C 432



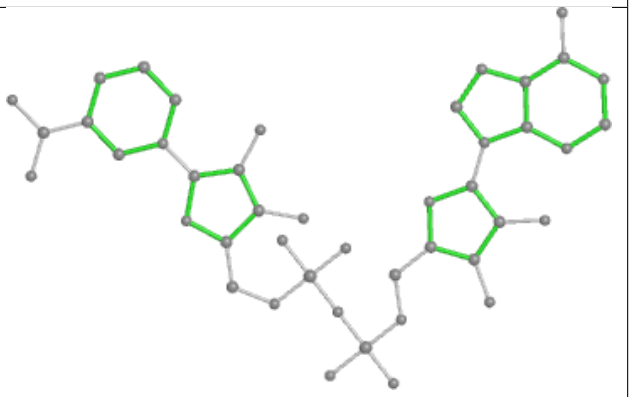
Bond lengths



Bond angles

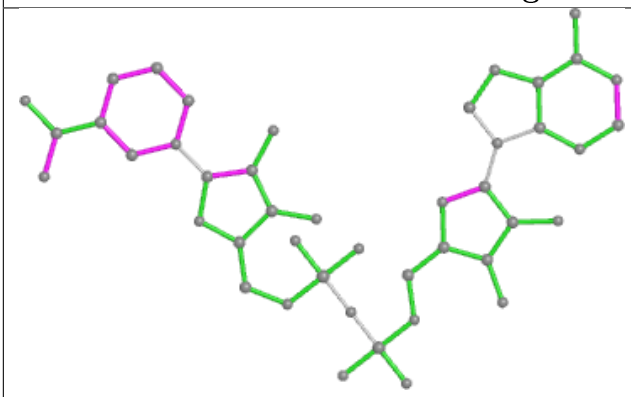


Torsions

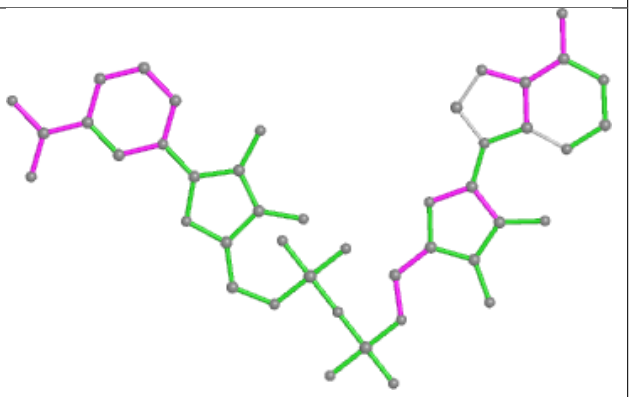


Rings

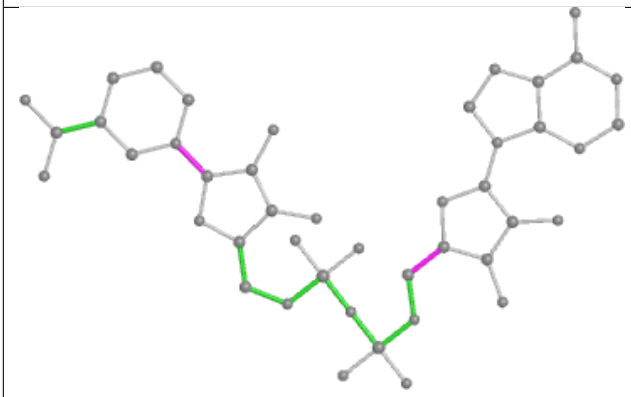
Ligand NAD F 432



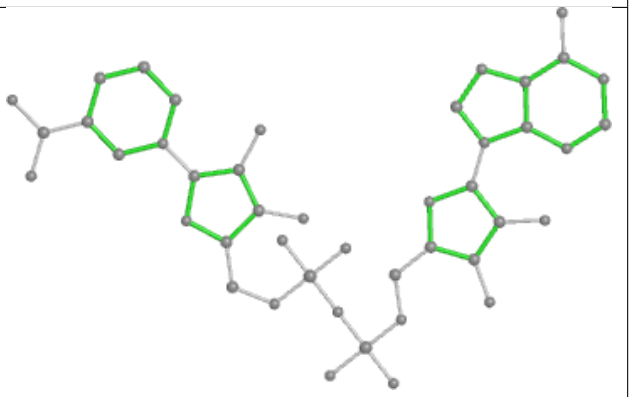
Bond lengths



Bond angles

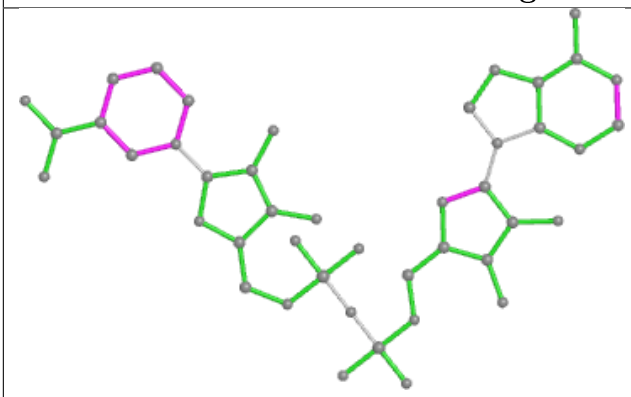


Torsions

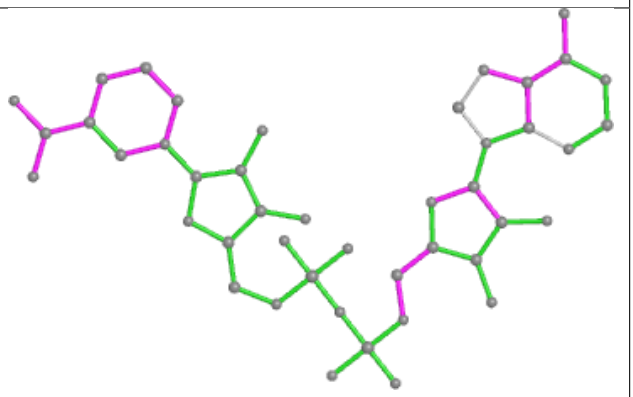


Rings

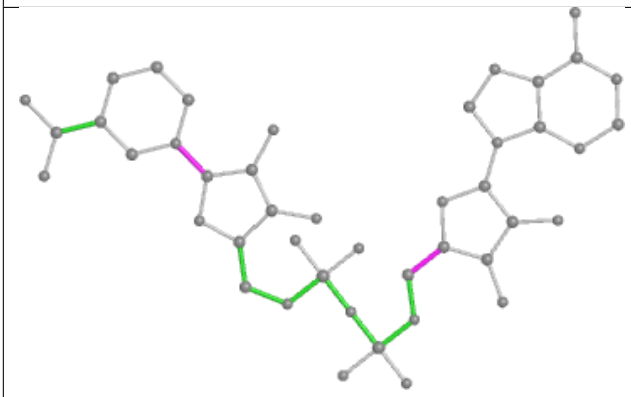
Ligand NAD A 432



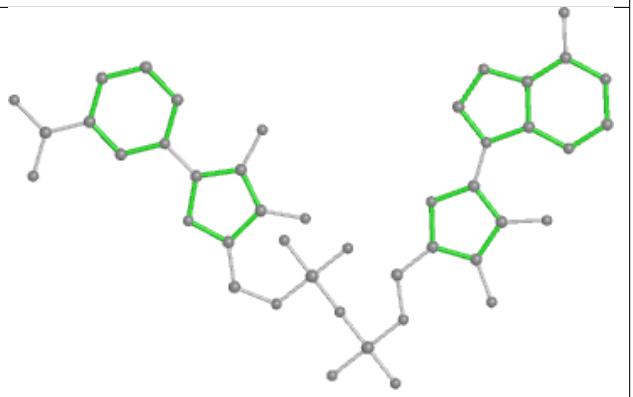
Bond lengths



Bond angles

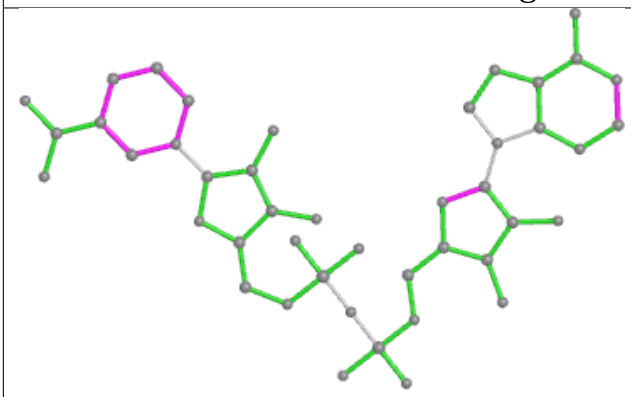


Torsions

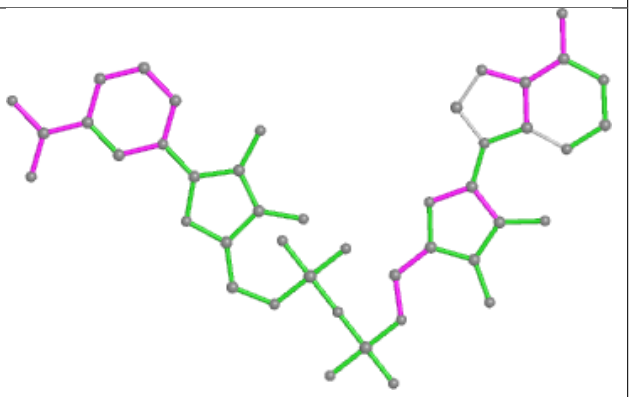


Rings

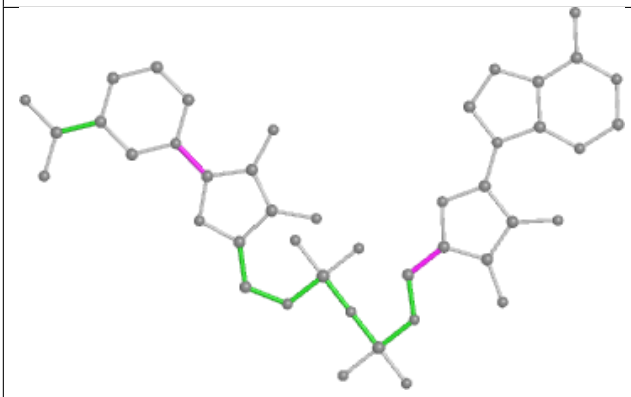
Ligand NAD D 432



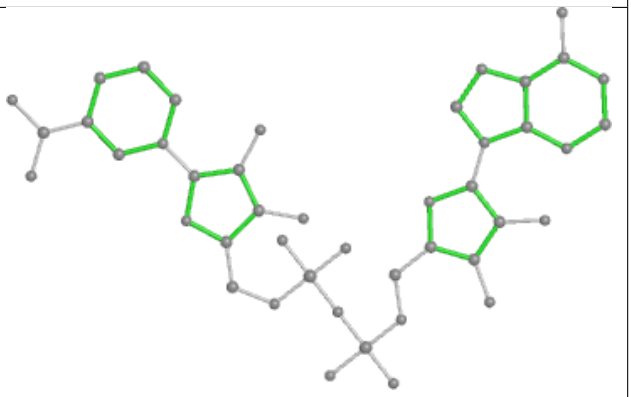
Bond lengths



Bond angles

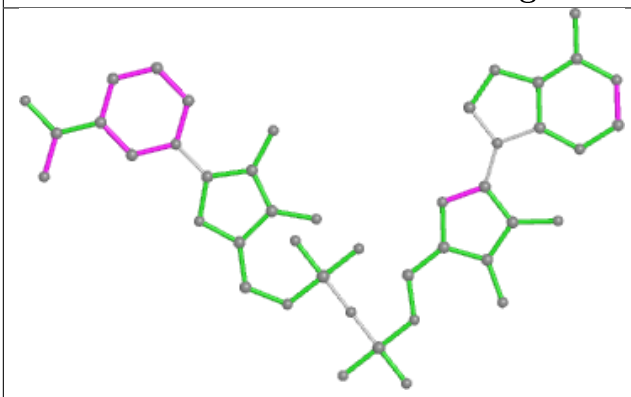


Torsions

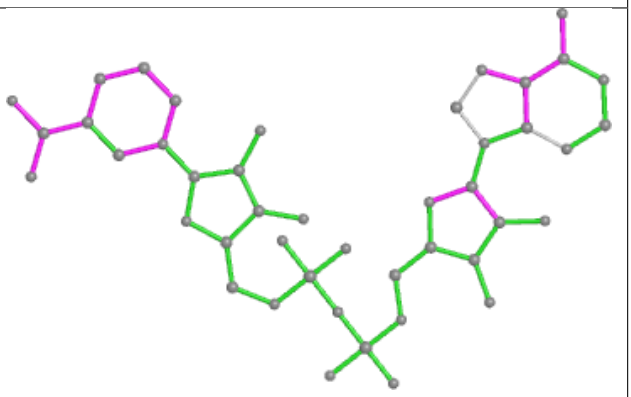


Rings

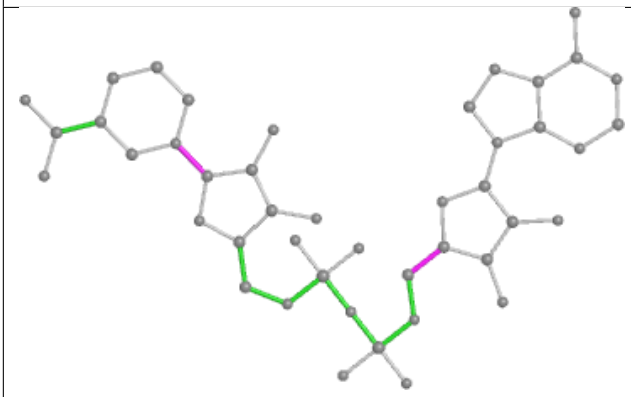
Ligand NAD G 432



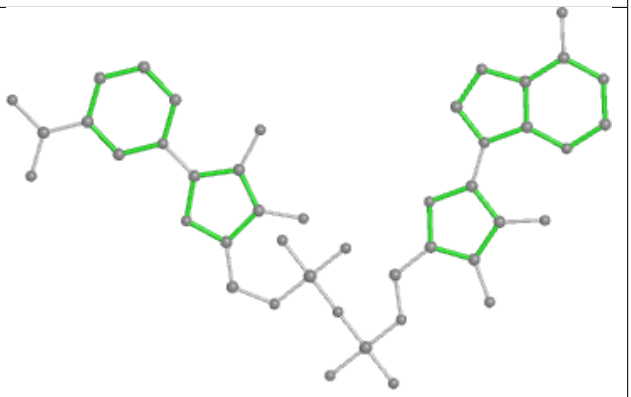
Bond lengths



Bond angles

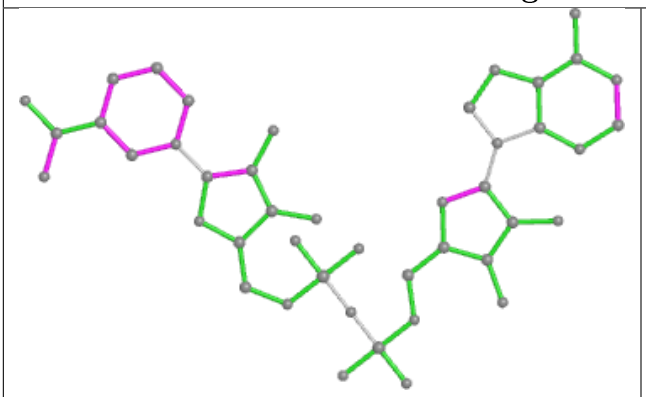


Torsions

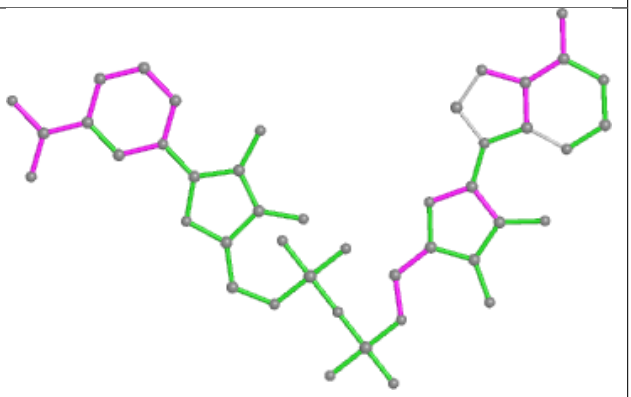


Rings

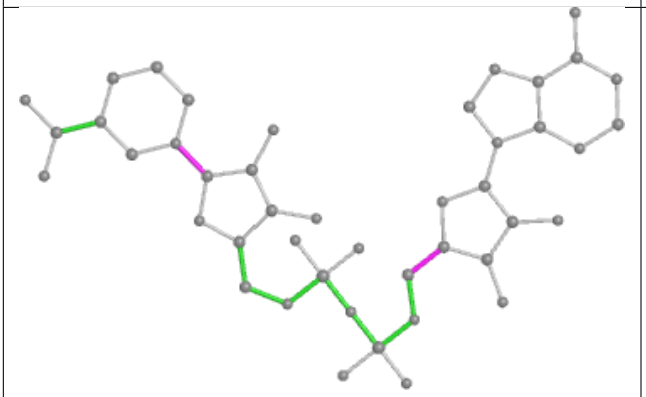
Ligand NAD E 432



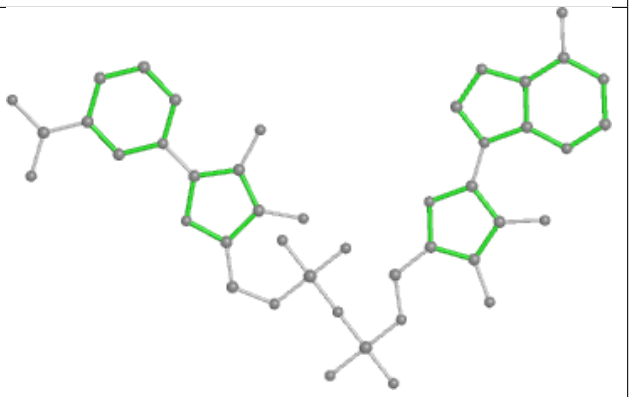
Bond lengths



Bond angles

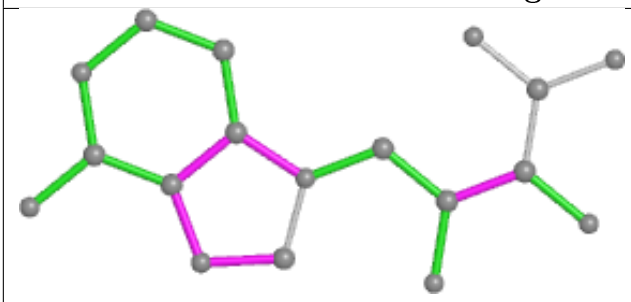


Torsions

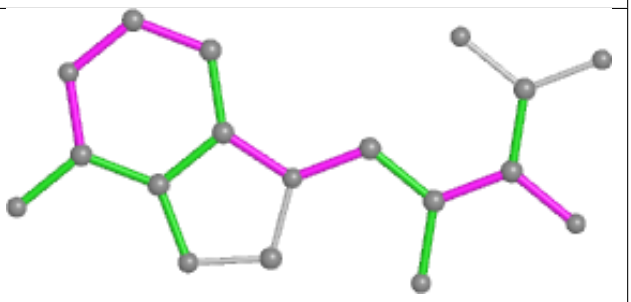


Rings

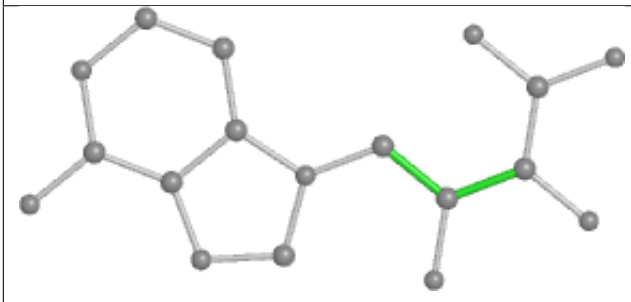
Ligand 3DD D 433



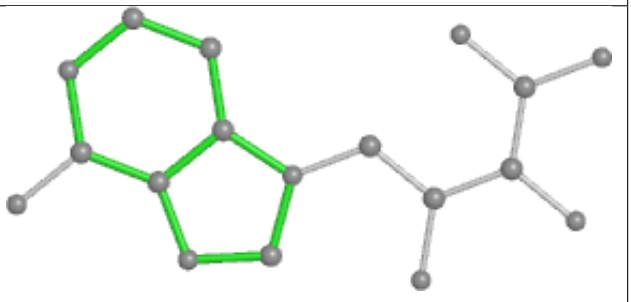
Bond lengths



Bond angles

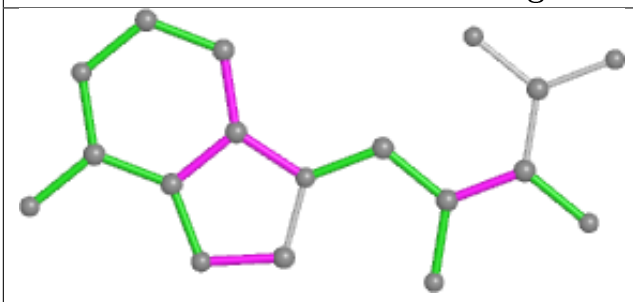


Torsions

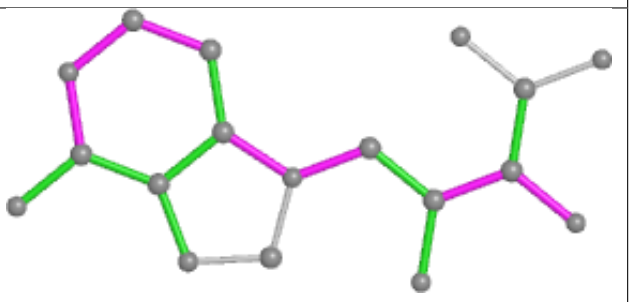


Rings

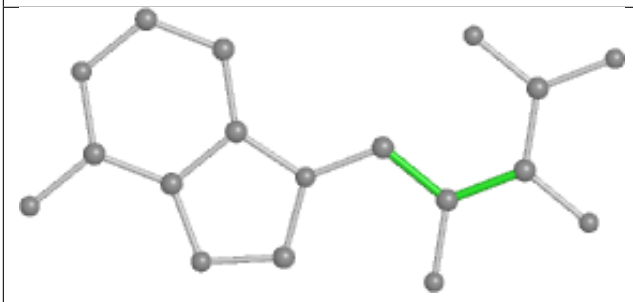
Ligand 3DD F 433



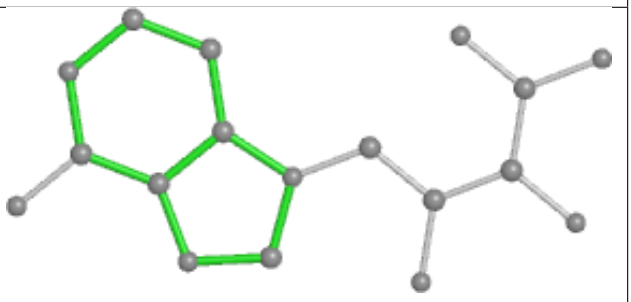
Bond lengths



Bond angles

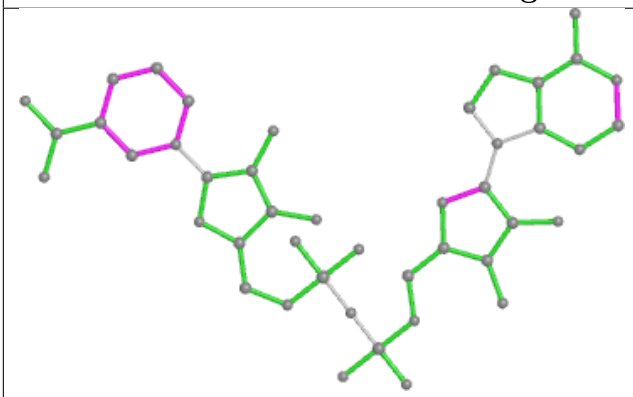


Torsions

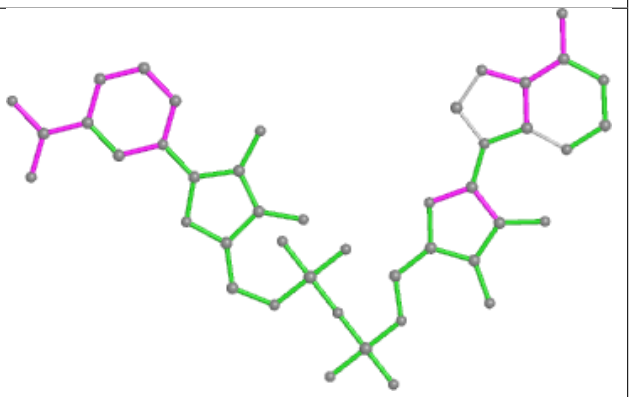


Rings

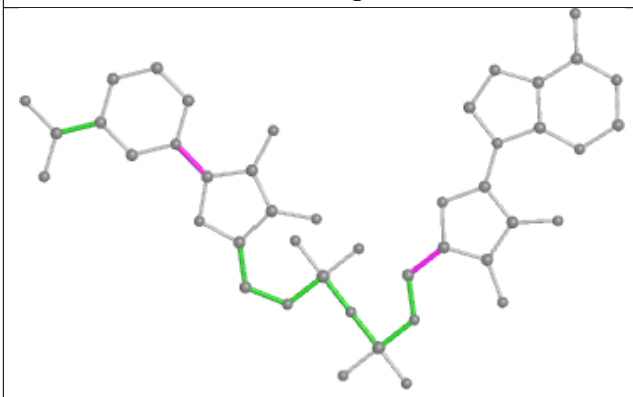
Ligand NAD B 432



Bond lengths



Bond angles



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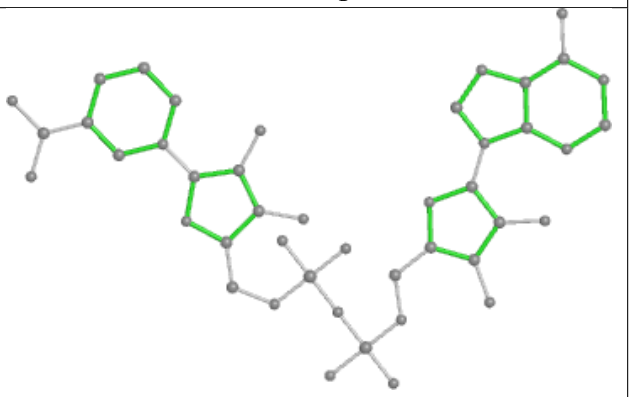
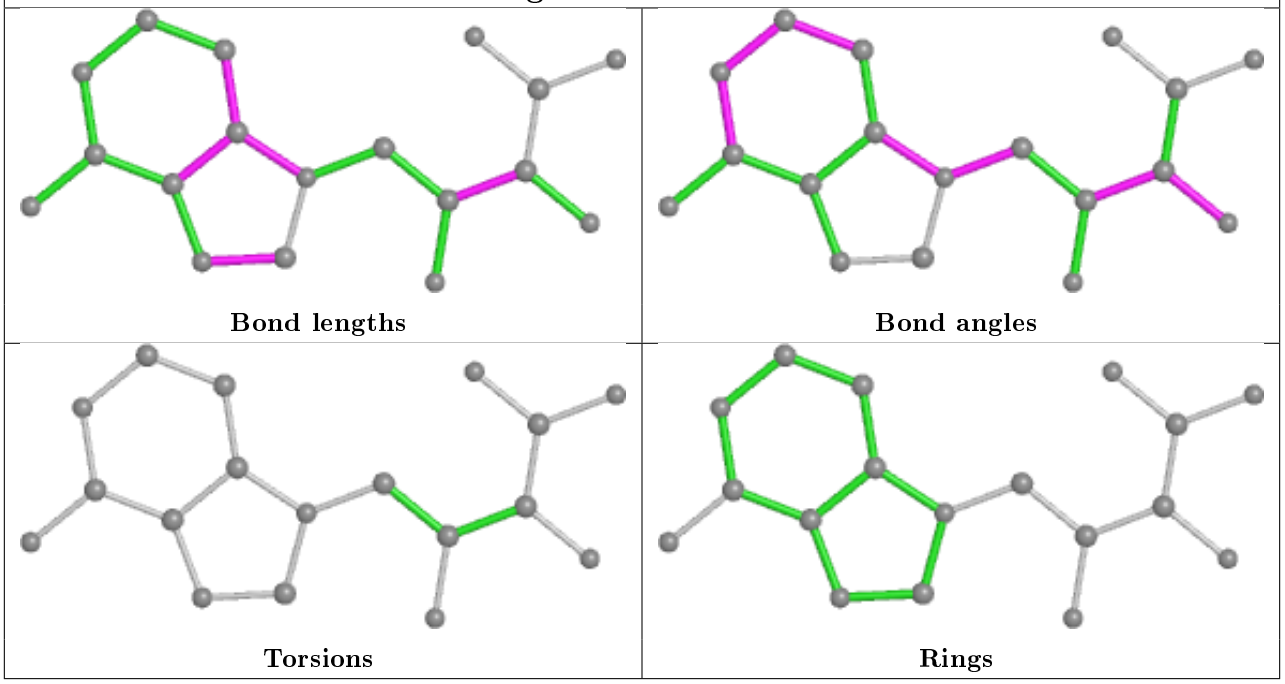
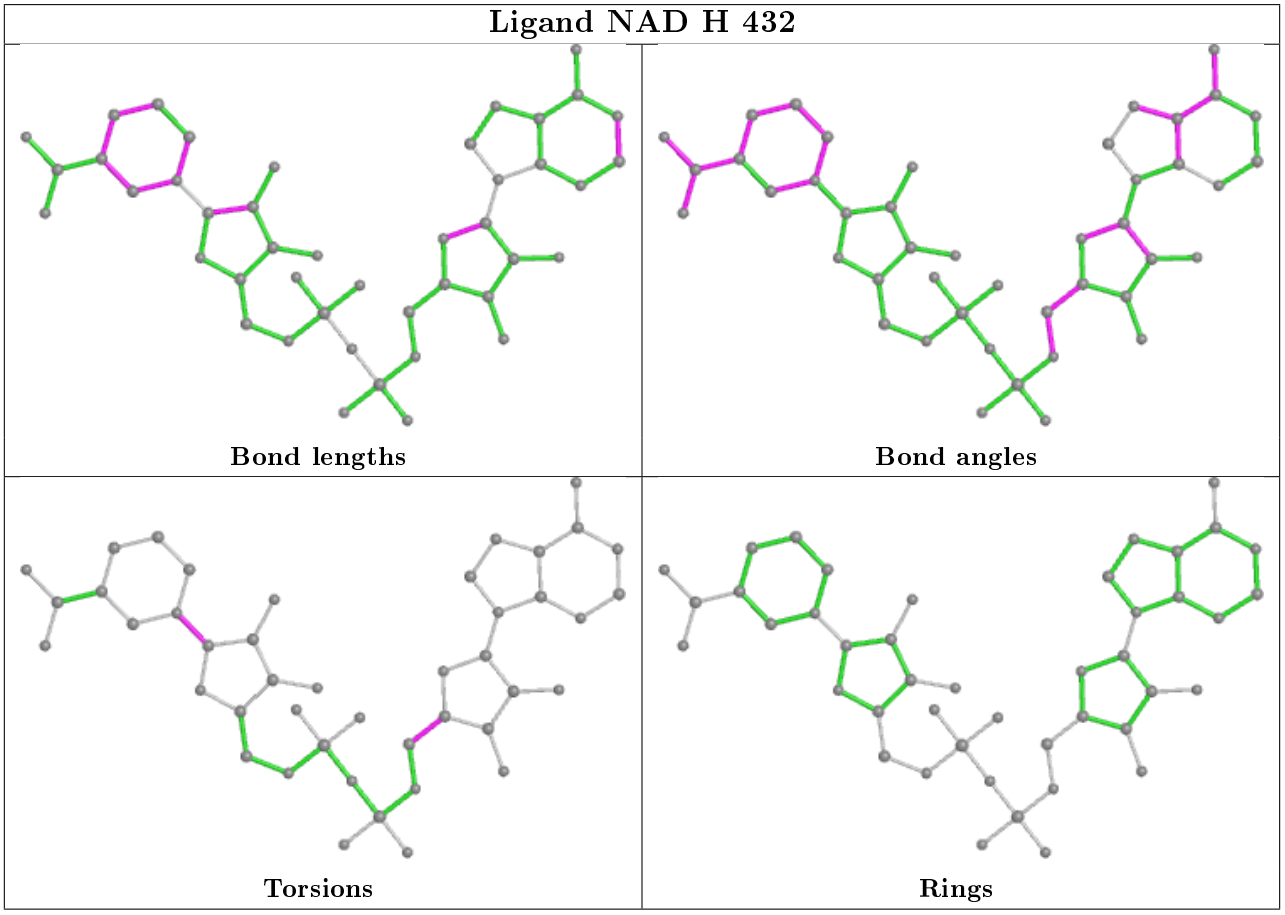


Rings

Ligand 3DD B 433



Ligand NAD H 432



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	430/431 (99%)	-0.67	2 (0%)	91 88	2, 4, 15, 39	0
1	B	430/431 (99%)	-0.56	4 (0%)	84 80	2, 5, 18, 44	0
1	C	430/431 (99%)	-0.44	5 (1%)	79 73	2, 5, 18, 44	0
1	D	430/431 (99%)	-0.25	16 (3%)	41 31	2, 5, 21, 43	0
1	E	430/431 (99%)	-0.64	3 (0%)	87 84	2, 4, 16, 39	0
1	F	430/431 (99%)	-0.66	2 (0%)	91 88	2, 4, 14, 43	0
1	G	430/431 (99%)	-0.56	3 (0%)	87 84	2, 5, 17, 44	0
1	H	430/431 (99%)	-0.63	1 (0%)	95 94	2, 4, 15, 40	0
All	All	3440/3448 (99%)	-0.55	36 (1%)	82 77	2, 4, 17, 44	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	ASP	8.1
1	F	2	ASP	7.3
1	G	2	ASP	6.8
1	B	2	ASP	6.4
1	D	2	ASP	4.4
1	D	5	PRO	4.2
1	G	376	ASP	4.2
1	E	2	ASP	4.1
1	F	3	LYS	4.0
1	C	3	LYS	3.5
1	G	3	LYS	3.5
1	A	2	ASP	3.3
1	D	116	THR	3.2
1	D	171	ILE	3.1
1	D	141	LYS	3.0
1	E	40	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	4	LEU	2.8
1	D	144	GLN	2.7
1	D	145	LEU	2.6
1	A	376	ASP	2.5
1	E	376	ASP	2.5
1	D	112	CYS	2.4
1	C	5	PRO	2.4
1	C	4	LEU	2.4
1	B	3	LYS	2.3
1	D	170	GLY	2.3
1	C	46	GLY	2.3
1	B	300	HIS	2.2
1	D	140	THR	2.2
1	D	106	ASP	2.2
1	D	9	ALA	2.1
1	D	4	LEU	2.1
1	D	122	GLY	2.1
1	H	147	SER	2.1
1	D	120	LYS	2.0
1	D	3	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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
3	3DD	H	433	18/18	0.90	0.16	2,3,6,9	0
3	3DD	F	433	18/18	0.91	0.16	2,2,8,9	0
3	3DD	B	433	18/18	0.91	0.14	2,2,8,14	0

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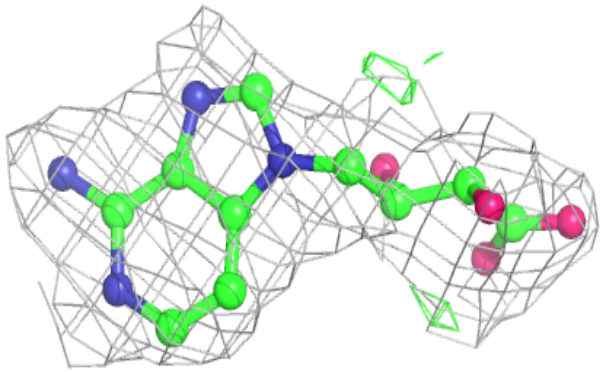
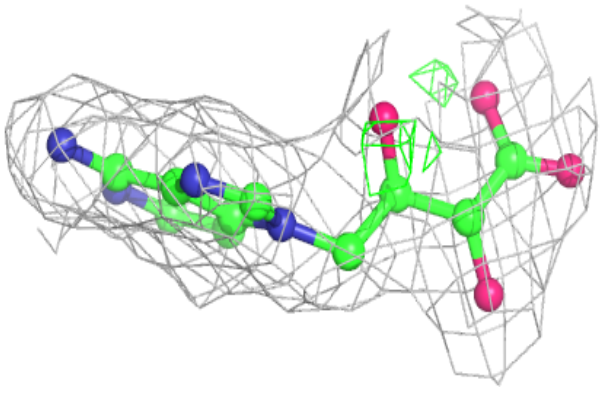
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	3DD	A	433	18/18	0.92	0.14	2,3,8,10	0
3	3DD	C	433	18/18	0.92	0.14	2,5,9,12	0
3	3DD	D	433	18/18	0.92	0.15	2,2,6,14	0
3	3DD	G	433	18/18	0.92	0.14	2,4,8,11	0
3	3DD	E	433	18/18	0.92	0.15	2,2,5,10	0
2	NAD	H	432	44/44	0.94	0.14	2,2,5,10	0
2	NAD	A	432	44/44	0.95	0.12	2,2,6,6	0
2	NAD	E	432	44/44	0.96	0.11	2,2,5,7	0
2	NAD	F	432	44/44	0.96	0.11	2,2,5,8	0
2	NAD	C	432	44/44	0.96	0.11	2,2,6,8	0
2	NAD	B	432	44/44	0.96	0.11	2,2,6,10	0
2	NAD	D	432	44/44	0.96	0.11	2,3,6,8	0
2	NAD	G	432	44/44	0.96	0.10	2,2,6,12	0

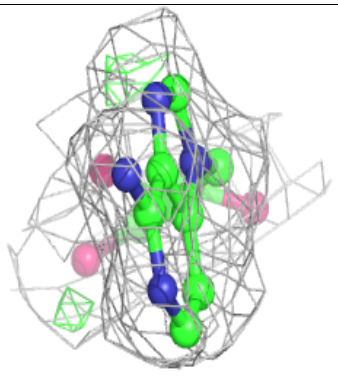
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3DD H 433:

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

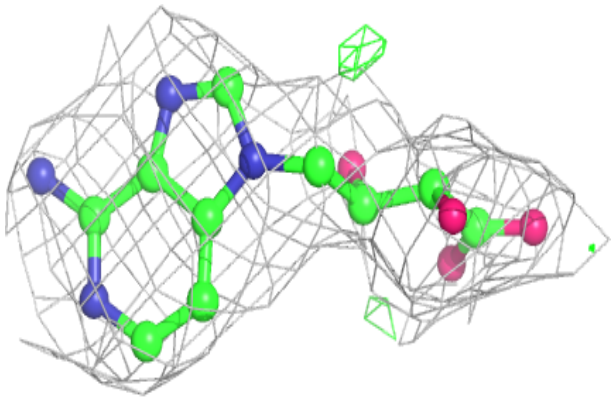


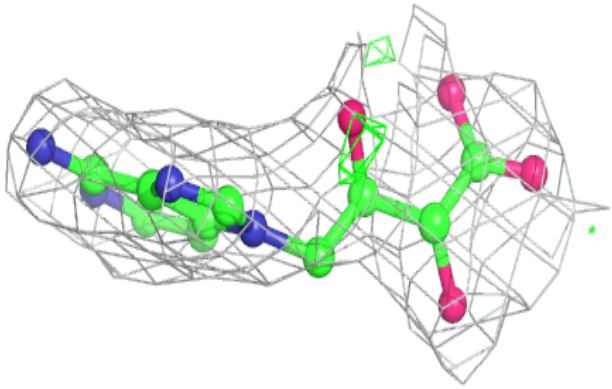


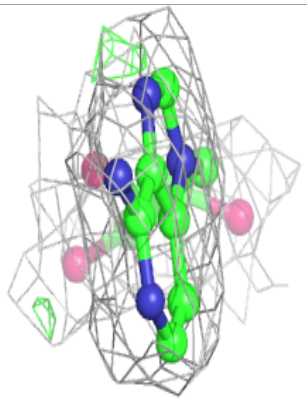


Electron density around 3DD F 433:

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

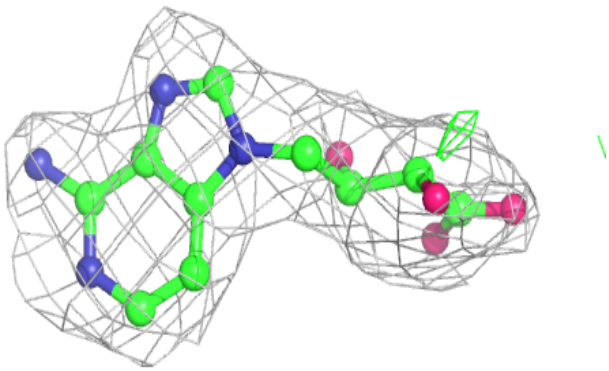


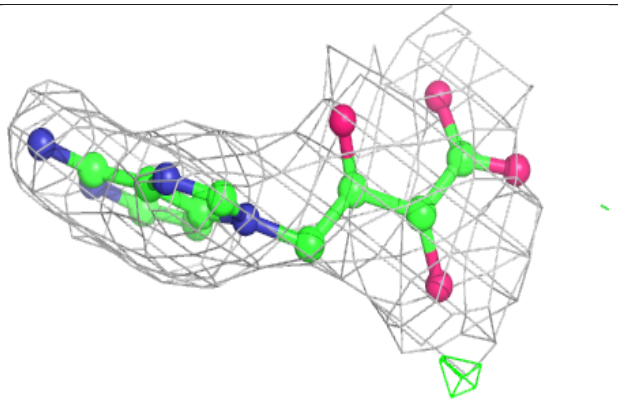


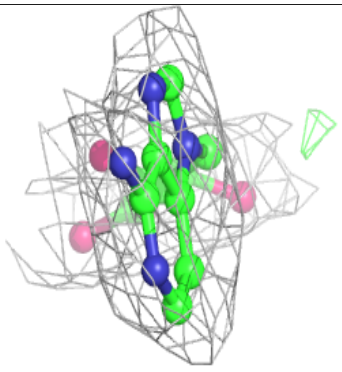


Electron density around 3DD B 433:

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

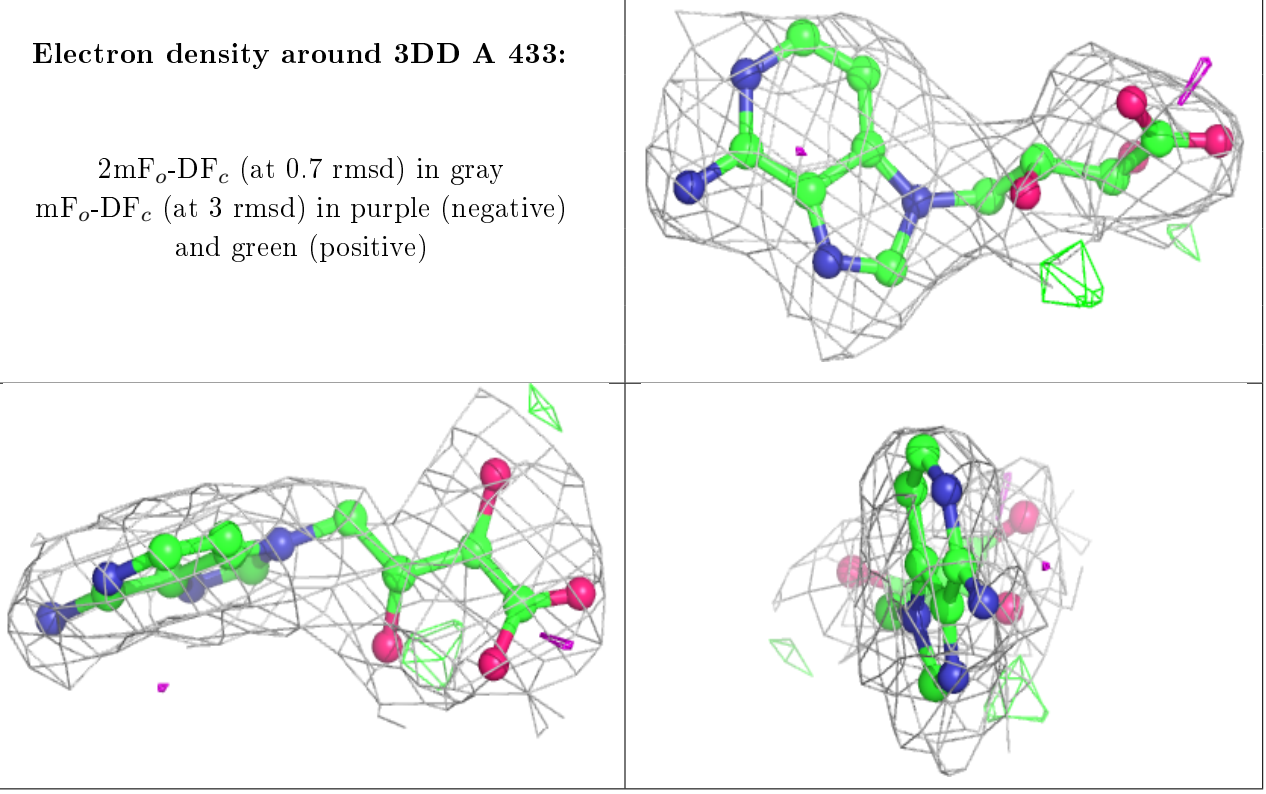






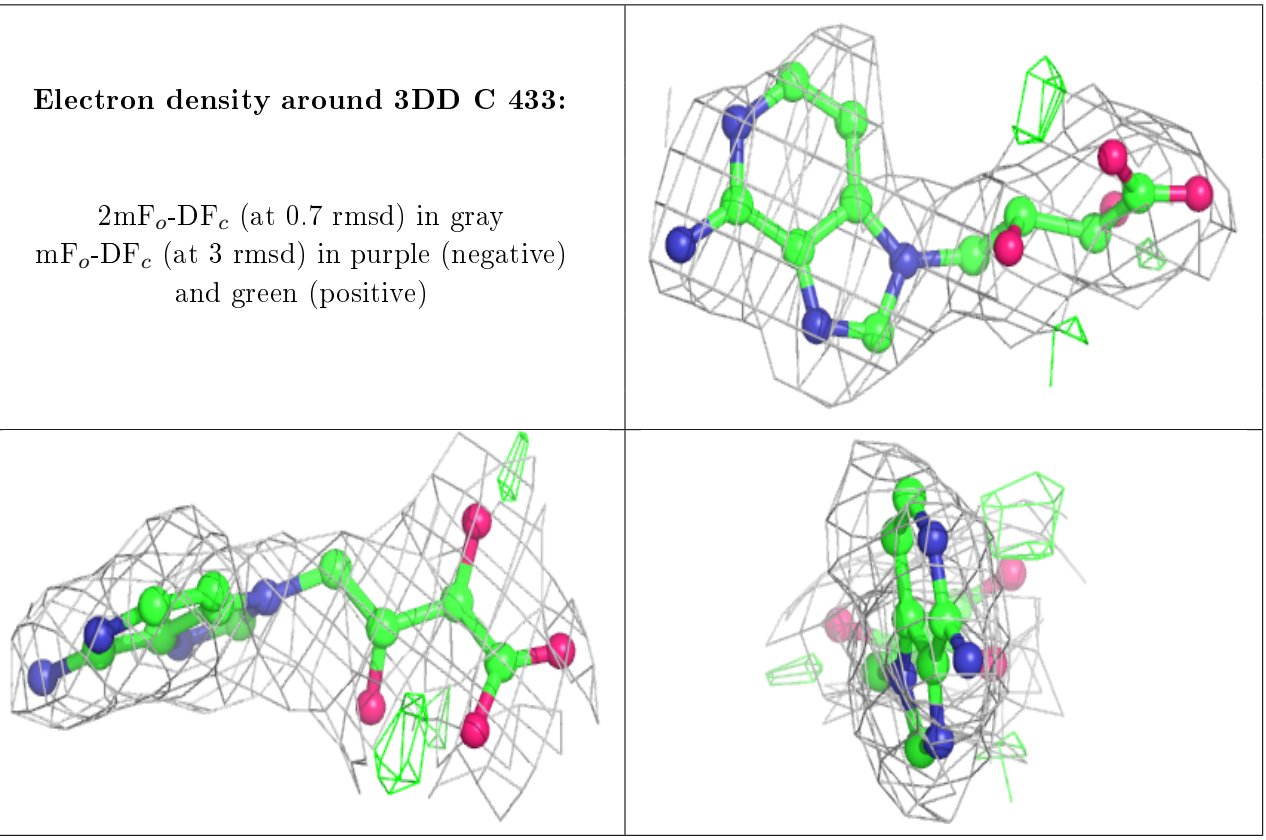
Electron density around 3DD A 433:

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



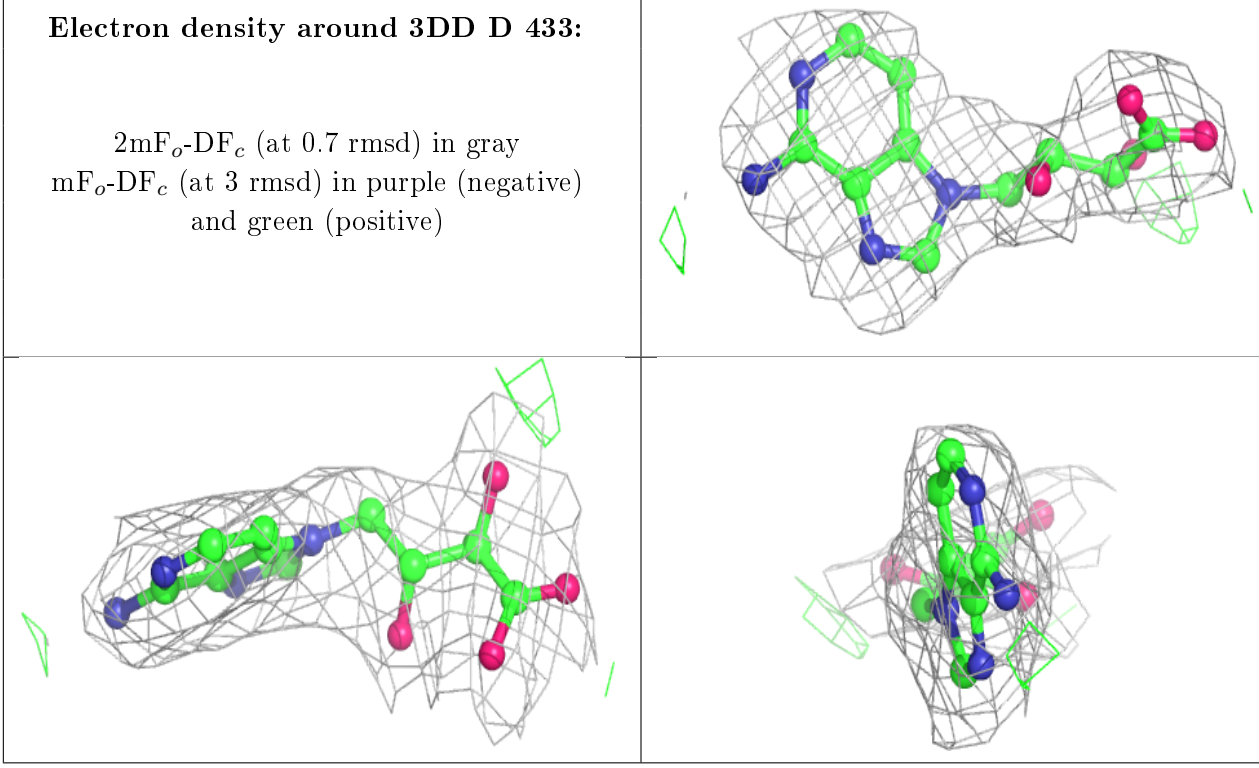
Electron density around 3DD C 433:

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



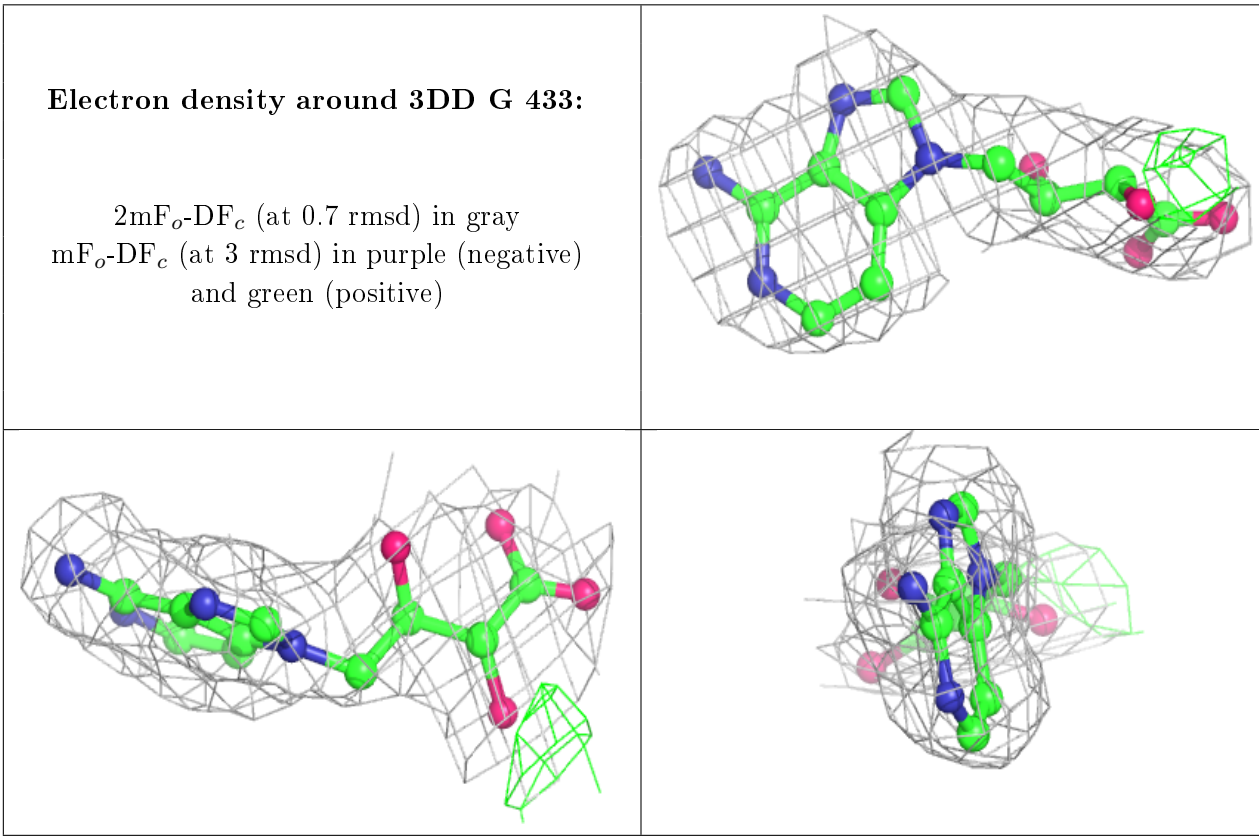
Electron density around 3DD D 433:

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



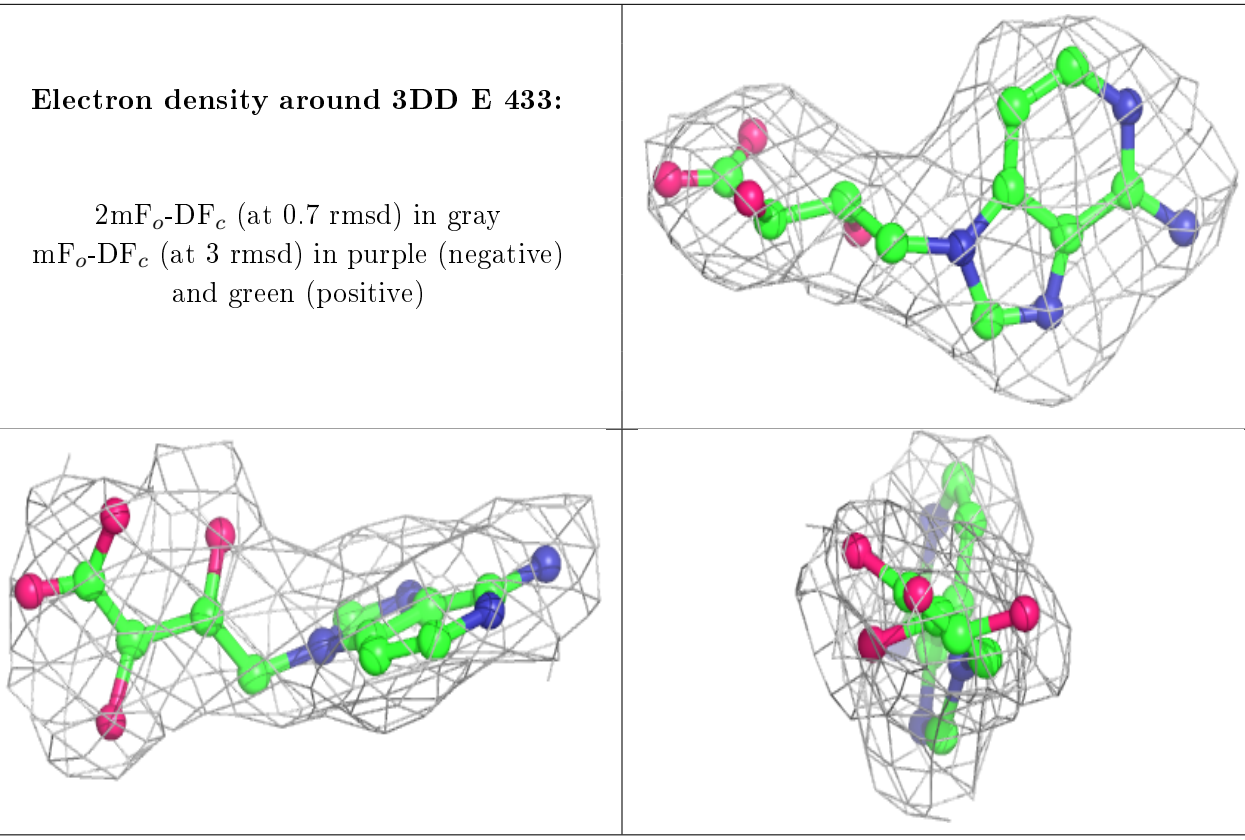
Electron density around 3DD G 433:

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



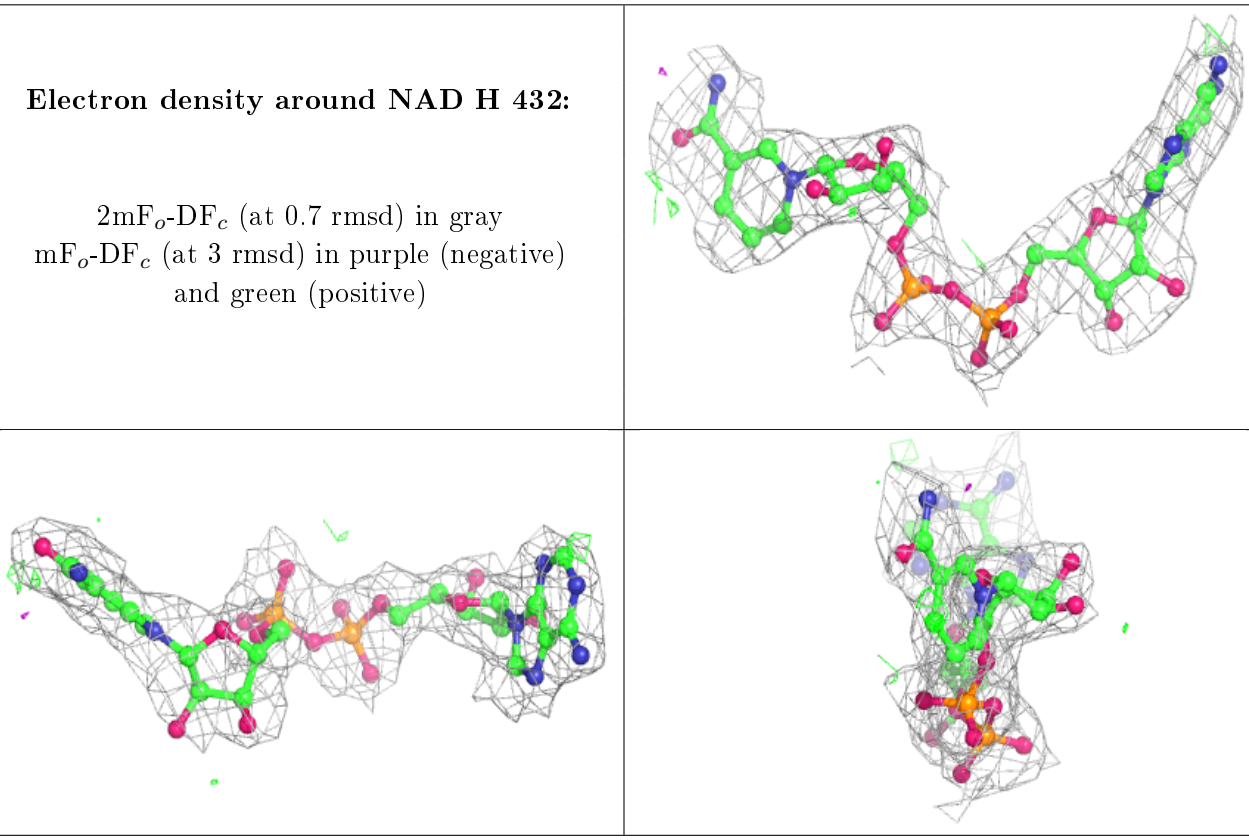
Electron density around 3DD E 433:

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



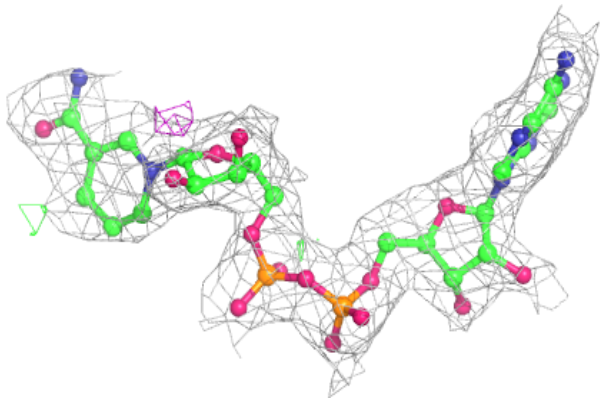
Electron density around NAD H 432:

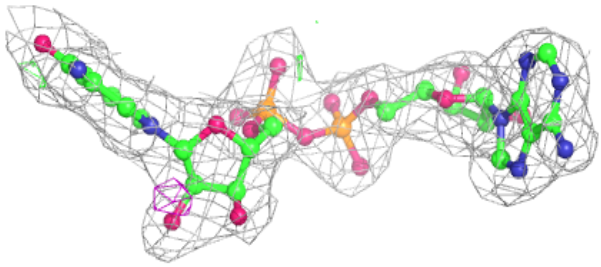
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

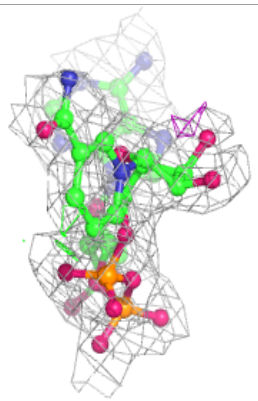


Electron density around NAD A 432:

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

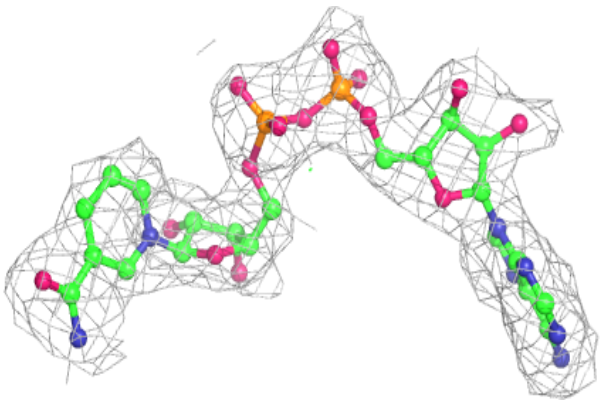


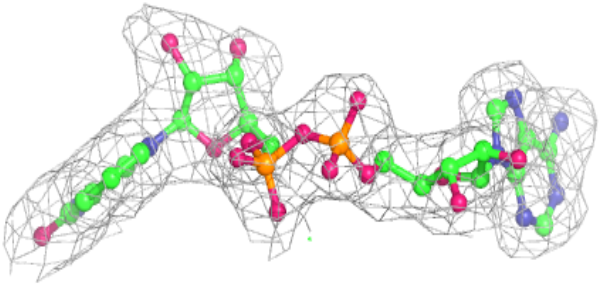


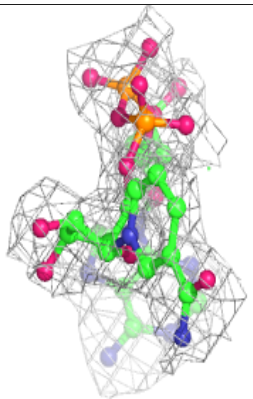


Electron density around NAD E 432:

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

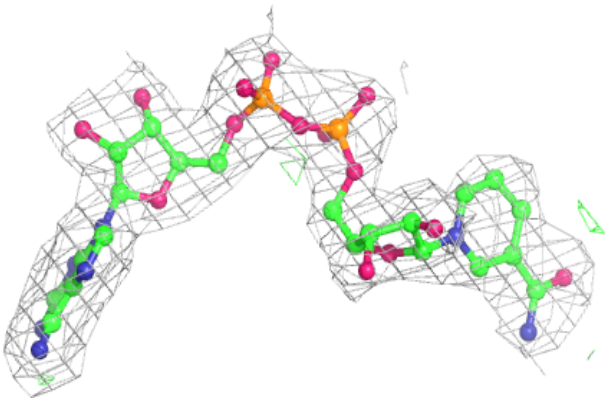


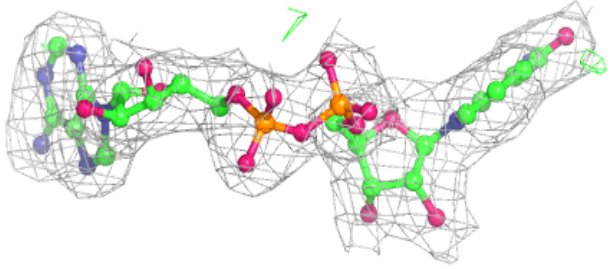


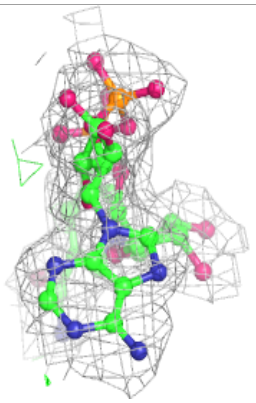


Electron density around NAD F 432:

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

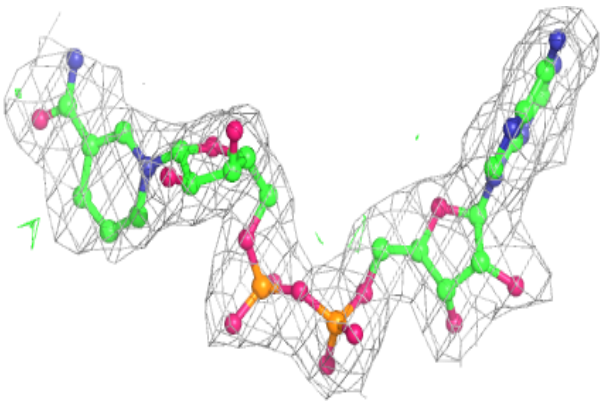


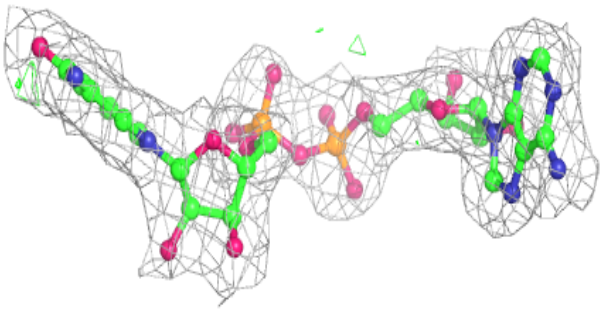


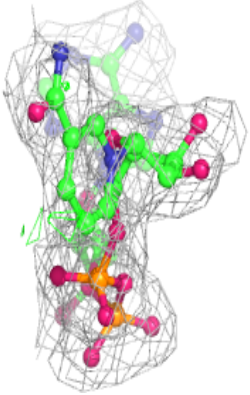


Electron density around NAD C 432:

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

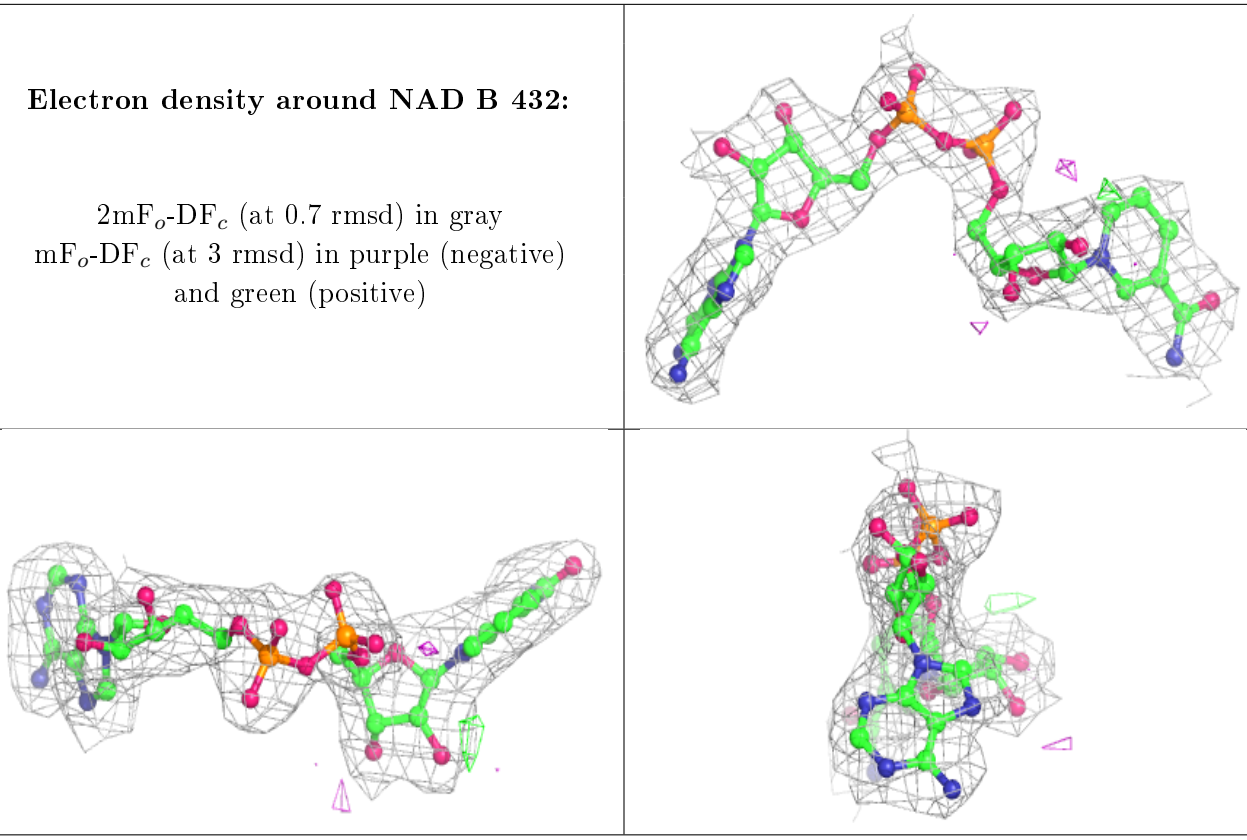






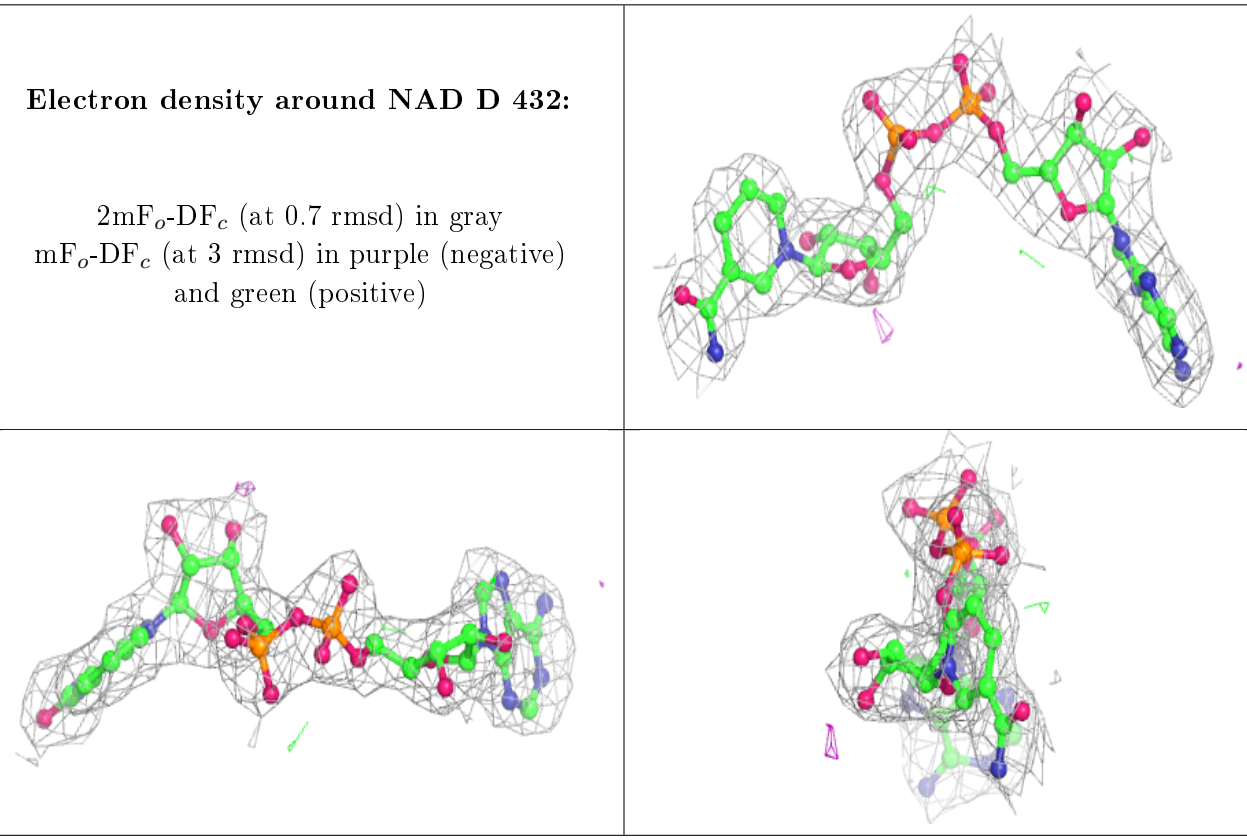
Electron density around NAD B 432:

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



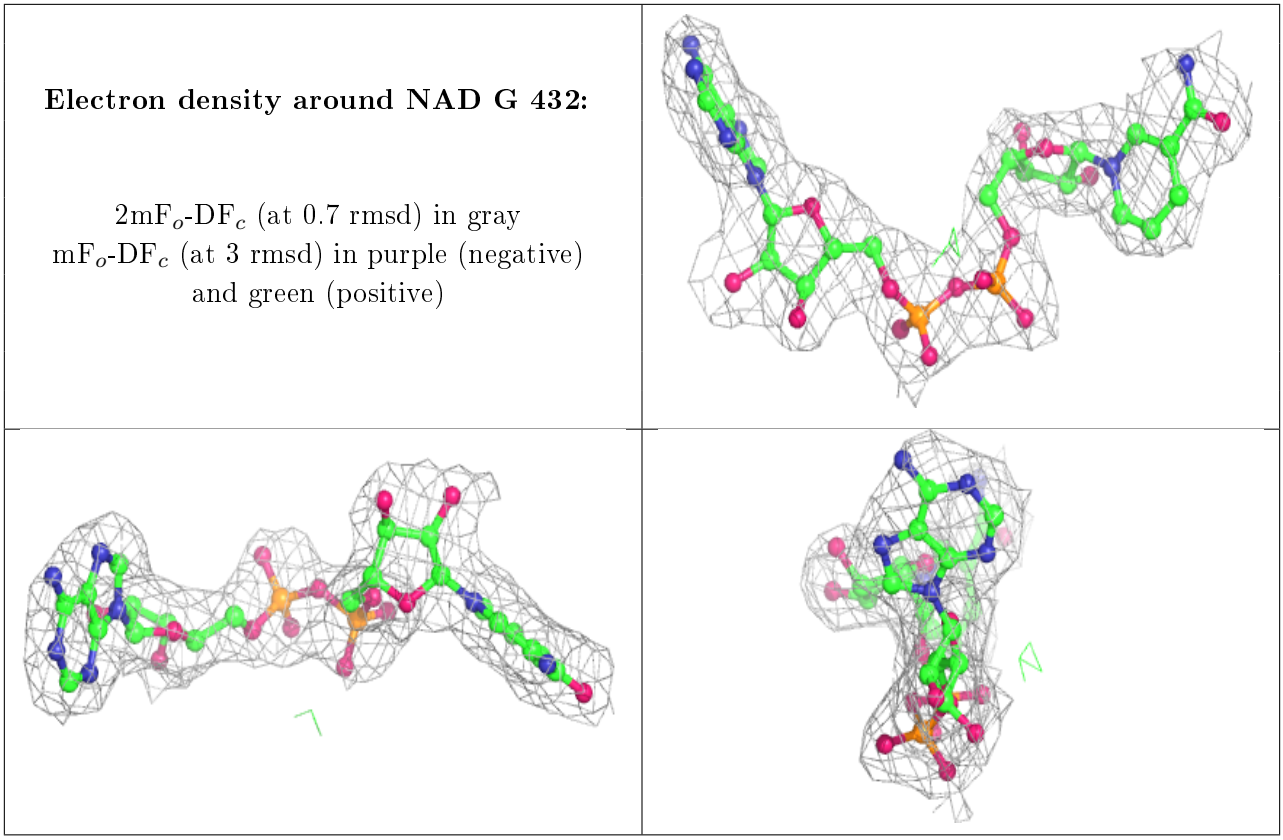
Electron density around NAD D 432:

$2mF_o$-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 432:

$2mF_o$-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.