



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:14 PM UTC

PDB ID : 1XWF / pdb_00001xwf
Title : K185N mutated S-adenosylhomocysteine hydrolase
Authors : Yamada, T.; Takata, Y.; Komoto, J.; Gomi, T.; Ogawa, H.; Fujioka, M.; Takusagawa, F.
Deposited on : 2004-11-01
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

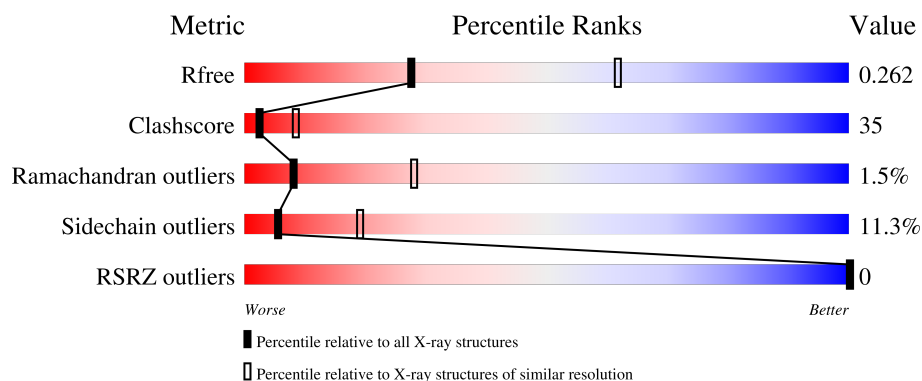
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	
1	B	431	
1	C	431	
1	D	431	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13564 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
			3318	2106	571	616	25			
1	B	430	Total	C	N	O	S	0	0	0
			3318	2106	571	616	25			
1	C	430	Total	C	N	O	S	0	0	0
			3318	2106	571	616	25			
1	D	430	Total	C	N	O	S	0	0	0
			3318	2106	571	616	25			

There are 4 discrepancies between the modelled and reference sequences:

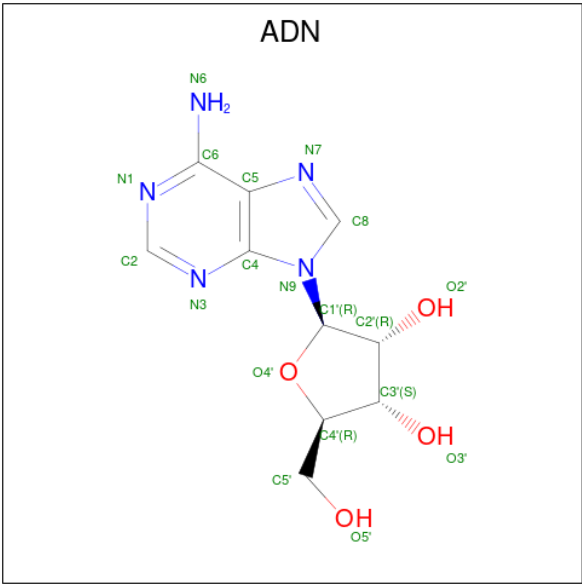
Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ASN	LYS	engineered mutation	UNP P10760
B	185	ASN	LYS	engineered mutation	UNP P10760
C	185	ASN	LYS	engineered mutation	UNP P10760
D	185	ASN	LYS	engineered mutation	UNP P10760

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: 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		

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		

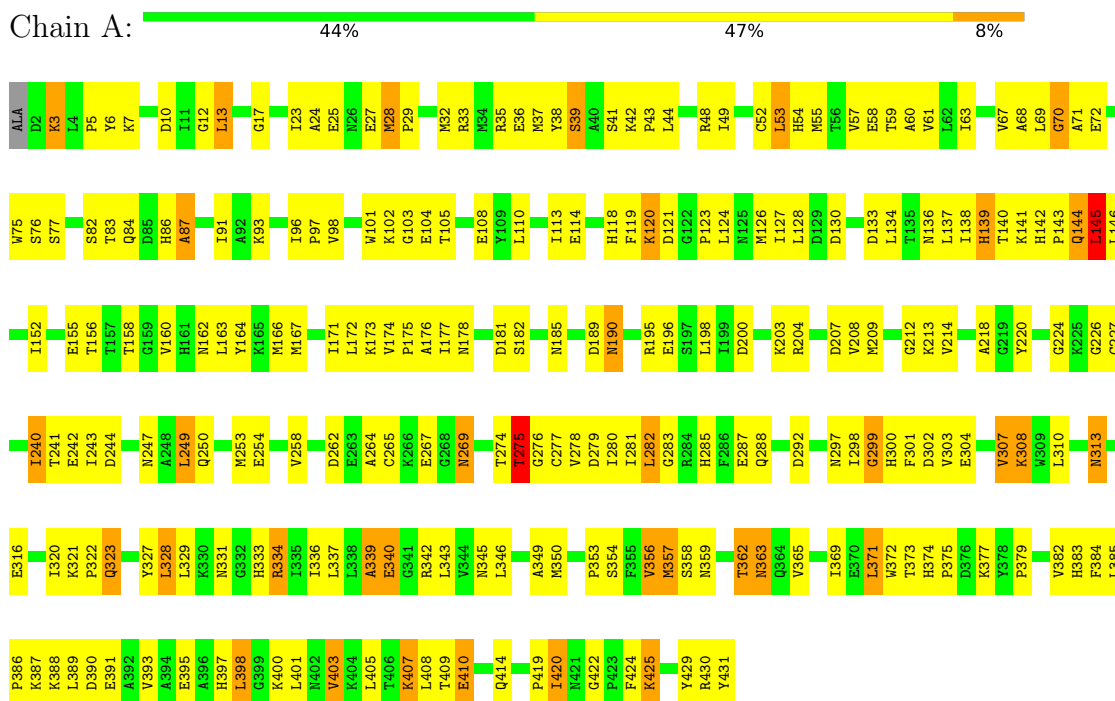
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	12	Total	O	0	0
			12	12		
4	C	11	Total	O	0	0
			11	11		
4	D	8	Total	O	0	0
			8	8		

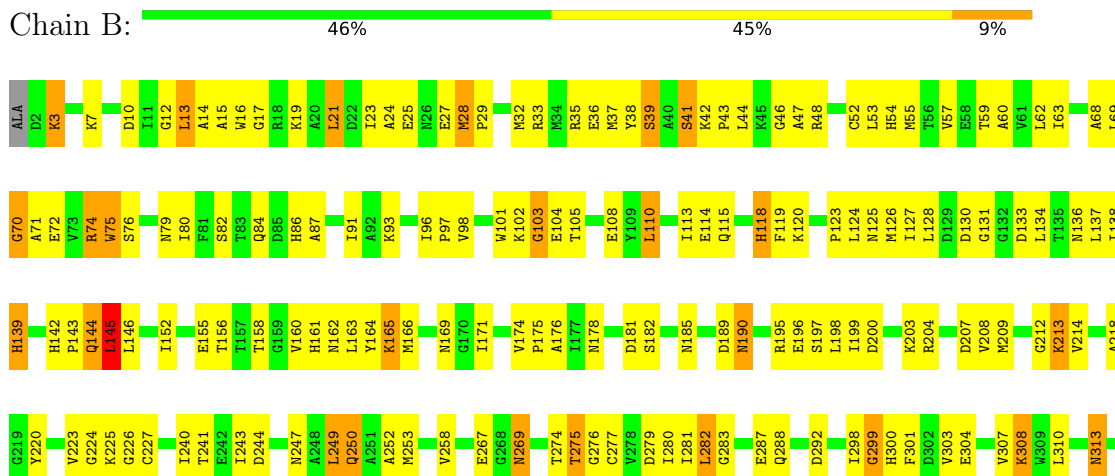
3 Residue-property plots

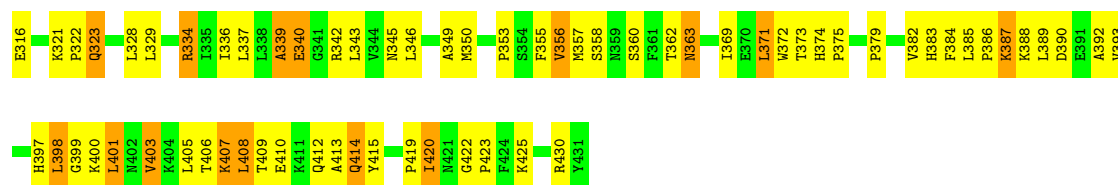
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Adenosylhomocysteinase



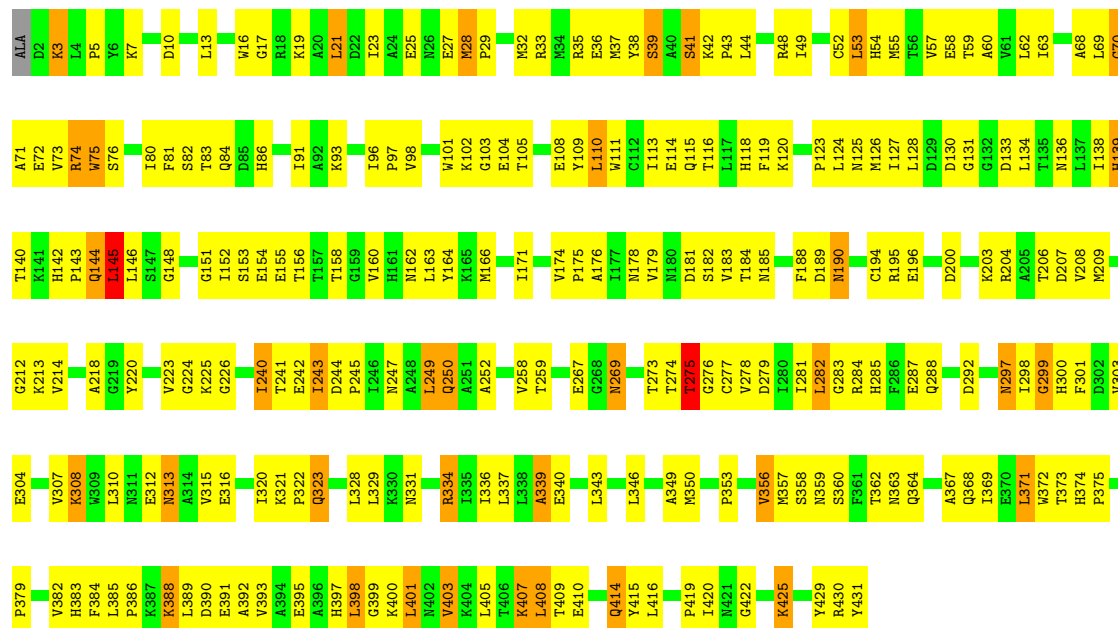
• Molecule 1: Adenosylhomocysteinase





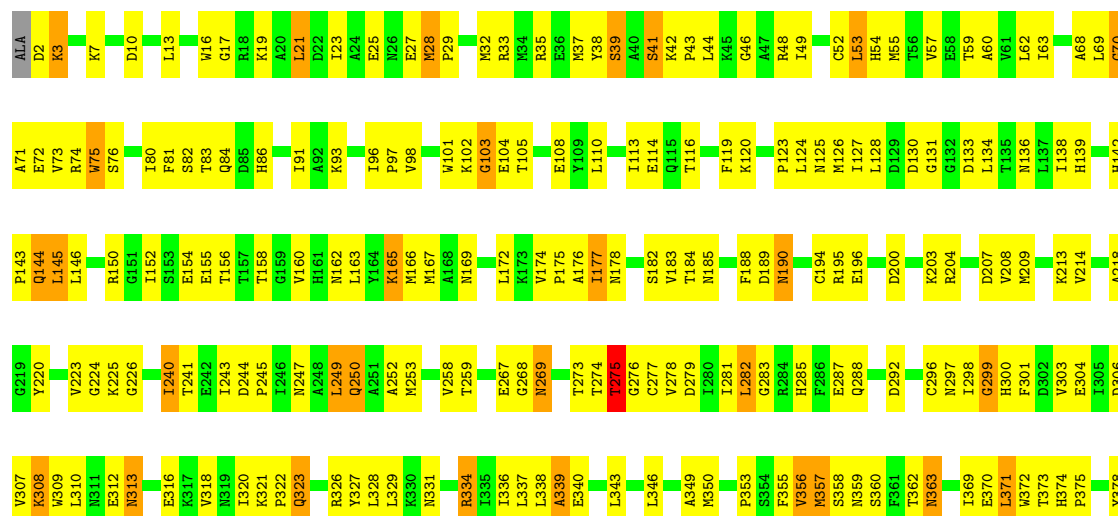
• Molecule 1: Adenosylhomocysteinase

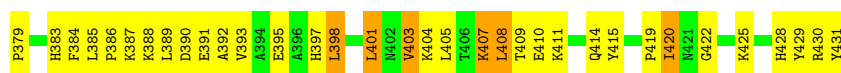
Chain C: 42% 49% 8%



• Molecule 1: Adenosylhomocysteinase

Chain D: 43% 48% 8%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.34Å 109.37Å 104.07Å 90.00° 115.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 98.8 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.286 0.207 , 0.262	Depositor DCC
R_{free} test set	4580 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 1.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.208 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13564	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	0/3383	1.02	19/4579 (0.4%)
1	B	0.56	0/3383	1.00	14/4579 (0.3%)
1	C	0.55	0/3383	1.01	17/4579 (0.4%)
1	D	0.56	0/3383	1.01	13/4579 (0.3%)
All	All	0.56	0/13532	1.01	63/18316 (0.3%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	SER	N-CA-C	-7.86	99.94	110.55
1	A	390	ASP	N-CA-C	-7.76	102.76	111.14
1	C	182	SER	N-CA-C	-7.72	100.13	110.55
1	C	362	THR	N-CA-C	-7.55	103.06	111.82
1	D	362	THR	N-CA-C	-7.41	103.23	111.82
1	A	28	MET	CA-C-N	7.12	126.95	119.05
1	A	28	MET	C-N-CA	7.12	126.95	119.05
1	D	182	SER	N-CA-C	-7.09	100.98	110.55
1	C	249	LEU	N-CA-C	-7.08	103.49	111.14
1	A	269	ASN	N-CA-C	-7.07	105.28	114.04
1	D	390	ASP	N-CA-C	-6.95	103.31	111.03
1	B	182	SER	N-CA-C	-6.88	101.26	110.55
1	C	269	ASN	N-CA-C	-6.78	105.63	114.04
1	D	269	ASN	N-CA-C	-6.66	105.79	114.04
1	A	145	LEU	N-CA-C	6.65	119.36	111.71
1	C	28	MET	CA-C-N	6.59	126.37	119.05
1	C	28	MET	C-N-CA	6.59	126.37	119.05
1	B	28	MET	CA-C-N	6.59	125.82	118.97
1	B	28	MET	C-N-CA	6.59	125.82	118.97
1	D	28	MET	CA-C-N	6.50	126.26	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	MET	C-N-CA	6.50	126.26	119.05
1	B	118	HIS	N-CA-C	6.19	119.03	109.07
1	C	390	ASP	N-CA-C	-6.14	104.51	111.14
1	C	425	LYS	N-CA-C	6.09	118.10	108.23
1	B	362	THR	N-CA-C	-6.08	104.58	112.23
1	D	240	ILE	N-CA-C	6.04	117.17	108.48
1	B	249	LEU	N-CA-C	-6.01	104.81	111.36
1	A	362	THR	N-CA-C	-5.96	104.72	112.23
1	C	243	ILE	N-CA-C	-5.95	106.45	113.42
1	D	275	THR	N-CA-C	5.88	118.79	110.14
1	A	249	LEU	N-CA-C	-5.81	104.87	111.14
1	C	275	THR	N-CA-C	5.81	118.67	110.14
1	A	118	HIS	N-CA-C	5.80	118.41	109.07
1	B	390	ASP	N-CA-C	-5.69	104.77	110.97
1	B	363	ASN	N-CA-C	-5.59	105.09	111.07
1	A	69	LEU	N-CA-C	-5.56	106.70	112.93
1	B	75	TRP	N-CA-C	5.53	118.71	110.14
1	B	69	LEU	N-CA-C	-5.50	106.88	113.21
1	A	240	ILE	N-CA-C	5.48	116.37	108.48
1	C	240	ILE	N-CA-C	5.47	116.36	108.48
1	C	145	LEU	N-CA-C	5.46	118.75	111.75
1	A	363	ASN	N-CA-C	-5.42	105.37	111.28
1	A	59	THR	N-CA-C	-5.40	105.55	111.82
1	B	269	ASN	N-CA-C	-5.34	107.41	114.04
1	A	275	THR	N-CA-C	5.34	117.98	109.81
1	B	87	ALA	N-CA-C	-5.34	105.37	111.14
1	D	363	ASN	N-CA-C	-5.33	105.47	111.28
1	C	140	THR	N-CA-C	5.30	119.91	113.38
1	D	69	LEU	N-CA-C	-5.30	107.00	112.93
1	B	145	LEU	N-CA-C	5.28	119.21	112.34
1	C	49	ILE	N-CA-C	5.25	115.82	108.89
1	A	49	ILE	N-CA-C	5.25	116.14	108.58
1	C	69	LEU	N-CA-C	-5.23	107.08	112.93
1	D	249	LEU	N-CA-C	-5.19	105.31	111.69
1	A	425	LYS	N-CA-C	5.18	117.57	108.82
1	C	75	TRP	N-CA-C	5.15	118.12	110.14
1	D	75	TRP	N-CA-C	5.14	117.95	109.72
1	A	140	THR	N-CA-C	5.14	119.65	113.17
1	A	264	ALA	N-CA-C	5.12	116.86	111.28
1	B	197	SER	N-CA-C	5.07	120.09	112.94
1	D	49	ILE	N-CA-C	5.07	115.88	108.58
1	A	87	ALA	N-CA-C	-5.03	105.70	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	HIS	N-CA-C	5.03	117.17	109.07

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	3318	0	3334	244	0
1	B	3318	0	3334	236	0
1	C	3318	0	3334	250	0
1	D	3318	0	3334	264	0
2	A	44	0	26	4	0
2	B	44	0	26	4	0
2	C	44	0	26	5	0
2	D	44	0	26	5	0
3	A	19	0	13	1	0
3	B	19	0	13	0	0
3	C	19	0	13	0	0
3	D	19	0	13	1	0
4	A	9	0	0	1	0
4	B	12	0	0	4	0
4	C	11	0	0	4	0
4	D	8	0	0	0	0
All	All	13564	0	13492	941	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 35.

All (941) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:PRO:HG2	1:C:422:GLY:HA3	1.36	1.06
1:A:419:PRO:HG2	1:A:422:GLY:HA3	1.38	1.03
1:B:419:PRO:HG2	1:B:422:GLY:HA3	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:PRO:HG2	1:D:422:GLY:HA3	1.42	0.99
1:D:353:PRO:HD2	1:D:356:VAL:HG11	1.44	0.99
1:A:127:ILE:HG23	1:A:134:LEU:HD12	1.45	0.98
1:A:214:VAL:H	1:A:269:ASN:HD22	1.11	0.97
1:A:247:ASN:HD21	1:B:425:LYS:HE2	1.31	0.96
1:B:353:PRO:HD2	1:B:356:VAL:HG11	1.46	0.95
1:B:136:ASN:HD21	1:B:162:ASN:HD21	1.15	0.95
1:C:127:ILE:HG23	1:C:134:LEU:HD12	1.46	0.94
1:C:41:SER:HB2	1:C:43:PRO:HD3	1.49	0.94
1:B:214:VAL:H	1:B:269:ASN:HD22	1.16	0.93
1:C:247:ASN:HD21	1:D:425:LYS:HE2	1.32	0.93
1:D:143:PRO:HA	1:D:146:LEU:HD23	1.50	0.92
1:D:41:SER:HB2	1:D:43:PRO:HD3	1.51	0.92
1:C:353:PRO:HD2	1:C:356:VAL:HG11	1.53	0.91
1:B:35:ARG:O	1:B:39:SER:HB2	1.69	0.91
1:C:247:ASN:HA	1:C:250:GLN:HE21	1.36	0.90
1:B:323:GLN:HG3	1:B:339:ALA:HA	1.54	0.90
1:C:214:VAL:H	1:C:269:ASN:HD22	1.19	0.89
1:A:323:GLN:HG3	1:A:339:ALA:HA	1.52	0.88
1:D:127:ILE:HG23	1:D:134:LEU:HD12	1.53	0.88
1:B:127:ILE:HG23	1:B:134:LEU:HD12	1.53	0.88
1:C:323:GLN:HG3	1:C:339:ALA:HA	1.53	0.88
1:D:247:ASN:HA	1:D:250:GLN:HE21	1.39	0.88
1:C:126:MET:HE2	1:C:372:TRP:HB2	1.56	0.87
1:A:247:ASN:HA	1:A:250:GLN:HE21	1.37	0.86
1:D:385:LEU:HD12	1:D:386:PRO:HD2	1.58	0.86
1:C:343:LEU:HD23	1:C:346:LEU:HD12	1.58	0.86
1:B:143:PRO:HA	1:B:146:LEU:HD23	1.57	0.86
1:A:136:ASN:HD21	1:A:162:ASN:HD21	1.24	0.85
1:D:323:GLN:HG3	1:D:339:ALA:HA	1.58	0.85
1:A:353:PRO:HD2	1:A:356:VAL:HG11	1.57	0.85
1:A:35:ARG:O	1:A:39:SER:HB2	1.76	0.84
1:B:142:HIS:HB3	1:B:145:LEU:HD12	1.59	0.84
1:A:419:PRO:CG	1:A:422:GLY:HA3	2.07	0.84
1:A:143:PRO:HA	1:A:146:LEU:HD23	1.59	0.83
1:D:35:ARG:O	1:D:39:SER:HB2	1.78	0.83
1:D:343:LEU:HD23	1:D:346:LEU:HD12	1.59	0.83
1:A:126:MET:HE2	1:A:372:TRP:HB2	1.61	0.82
1:C:110:LEU:O	1:C:114:GLU:HG3	1.79	0.82
1:A:60:ALA:HA	1:A:91:ILE:HD11	1.62	0.82
1:D:136:ASN:HD21	1:D:162:ASN:HD21	1.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:VAL:H	1:D:269:ASN:HD22	1.28	0.82
1:D:353:PRO:O	1:D:356:VAL:HG13	1.80	0.81
1:A:425:LYS:HE2	1:B:247:ASN:HD21	1.46	0.81
1:B:247:ASN:HA	1:B:250:GLN:HE21	1.45	0.81
1:B:161:HIS:HB2	4:B:443:HOH:O	1.81	0.81
1:B:343:LEU:HD23	1:B:346:LEU:HD12	1.63	0.80
1:C:136:ASN:HD21	1:C:162:ASN:HD21	1.29	0.80
1:C:143:PRO:HA	1:C:146:LEU:HD23	1.61	0.80
1:B:419:PRO:CG	1:B:422:GLY:HA3	2.11	0.80
1:C:419:PRO:CG	1:C:422:GLY:HA3	2.10	0.79
1:A:142:HIS:HB3	1:A:145:LEU:HD12	1.64	0.79
1:C:385:LEU:HD12	1:C:386:PRO:HD2	1.63	0.79
1:B:156:THR:HA	4:B:435:HOH:O	1.83	0.78
1:B:385:LEU:HD12	1:B:386:PRO:HD2	1.64	0.78
1:A:41:SER:HB2	1:A:43:PRO:HD3	1.65	0.78
1:D:60:ALA:HA	1:D:91:ILE:HD11	1.66	0.78
1:A:430:ARG:HD3	1:B:430:ARG:HA	1.66	0.77
1:C:244:ASP:HB3	1:C:247:ASN:HD22	1.50	0.77
1:C:419:PRO:HG2	1:C:422:GLY:CA	2.13	0.77
1:D:419:PRO:CG	1:D:422:GLY:HA3	2.15	0.77
1:A:156:THR:O	1:A:160:VAL:HG23	1.85	0.77
1:B:142:HIS:HB3	1:B:145:LEU:CD1	2.15	0.76
1:C:292:ASP:OD1	1:C:336:ILE:HD11	1.85	0.76
1:A:292:ASP:OD1	1:A:336:ILE:HD11	1.84	0.76
1:B:209:MET:HE2	1:D:196:GLU:HG3	1.67	0.76
1:C:60:ALA:HA	1:C:91:ILE:HD11	1.67	0.76
1:A:110:LEU:O	1:A:114:GLU:HG3	1.86	0.76
1:C:35:ARG:O	1:C:39:SER:HB2	1.86	0.75
1:A:419:PRO:HG2	1:A:422:GLY:CA	2.14	0.75
1:B:292:ASP:OD1	1:B:336:ILE:HD11	1.87	0.74
1:A:385:LEU:HD12	1:A:386:PRO:HD2	1.70	0.74
1:B:130:ASP:O	1:B:156:THR:HG21	1.86	0.74
1:B:60:ALA:HA	1:B:91:ILE:HD11	1.70	0.73
1:B:393:VAL:O	1:B:397:HIS:HD2	1.70	0.73
1:D:353:PRO:HD2	1:D:356:VAL:CG1	2.17	0.73
1:B:41:SER:HB2	1:B:43:PRO:HD3	1.70	0.73
1:B:57:VAL:HG23	1:B:84:GLN:NE2	2.04	0.72
1:B:75:TRP:HH2	1:B:128:LEU:HD13	1.54	0.72
1:D:419:PRO:HG2	1:D:422:GLY:CA	2.16	0.72
1:A:142:HIS:HB3	1:A:145:LEU:CD1	2.18	0.72
1:C:190:ASN:N	1:C:190:ASN:HD22	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HG	1:A:403:VAL:CG2	2.21	0.71
1:C:247:ASN:ND2	1:D:425:LYS:HE2	2.05	0.71
1:D:275:THR:HG22	1:D:276:GLY:H	1.56	0.71
1:D:343:LEU:CD2	1:D:346:LEU:HD12	2.21	0.70
1:B:398:LEU:HG	1:B:403:VAL:CG2	2.21	0.70
1:B:203:LYS:O	1:B:207:ASP:N	2.24	0.70
1:C:353:PRO:O	1:C:356:VAL:HG13	1.91	0.70
1:C:258:VAL:HB	1:D:403:VAL:HB	1.74	0.70
1:C:105:THR:OG1	1:C:108:GLU:HG3	1.91	0.70
1:B:110:LEU:O	1:B:114:GLU:HG3	1.92	0.69
1:B:419:PRO:HG2	1:B:422:GLY:CA	2.19	0.69
1:A:430:ARG:HA	1:B:430:ARG:HD3	1.73	0.69
1:D:220:TYR:CD1	1:D:240:ILE:HD13	2.28	0.69
1:D:292:ASP:OD1	1:D:336:ILE:HD11	1.93	0.69
1:B:213:LYS:NZ	4:B:436:HOH:O	2.25	0.69
1:C:247:ASN:HA	1:C:250:GLN:NE2	2.07	0.69
1:C:308:LYS:H	1:C:308:LYS:HD2	1.57	0.69
1:C:386:PRO:HG2	1:C:389:LEU:HD12	1.75	0.69
1:C:425:LYS:HE2	1:D:247:ASN:HD21	1.57	0.69
1:A:353:PRO:O	1:A:356:VAL:HG13	1.93	0.68
1:B:300:HIS:HA	1:B:343:LEU:HD11	1.75	0.68
1:A:220:TYR:CD1	1:A:240:ILE:HD13	2.29	0.68
1:A:301:PHE:C	1:A:303:VAL:H	2.00	0.68
1:D:142:HIS:HB3	1:D:145:LEU:HD12	1.76	0.68
1:D:185:ASN:ND2	1:D:360:SER:HB2	2.09	0.67
1:D:247:ASN:HA	1:D:250:GLN:NE2	2.10	0.67
1:B:386:PRO:HG2	1:B:389:LEU:HD12	1.77	0.67
1:A:247:ASN:ND2	1:B:425:LYS:HE2	2.07	0.67
1:B:209:MET:CE	1:D:196:GLU:HG3	2.25	0.67
1:B:281:ILE:C	1:B:282:LEU:HD13	2.20	0.67
1:D:10:ASP:HB3	1:D:13:LEU:HD23	1.77	0.67
1:D:142:HIS:HB3	1:D:145:LEU:CD1	2.24	0.67
1:A:275:THR:HG21	2:A:432:NAD:C8A	2.25	0.66
1:A:343:LEU:HD23	1:A:346:LEU:HD12	1.77	0.66
1:B:308:LYS:H	1:B:308:LYS:HD2	1.60	0.66
1:B:283:GLY:O	1:B:287:GLU:HG3	1.96	0.66
1:B:353:PRO:HD2	1:B:356:VAL:CG1	2.24	0.66
1:A:393:VAL:O	1:A:397:HIS:HD2	1.79	0.66
1:A:105:THR:OG1	1:A:108:GLU:HG3	1.95	0.65
1:A:127:ILE:CG2	1:A:134:LEU:HD12	2.24	0.65
1:A:17:GLY:HA2	1:A:86:HIS:HD2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:CD2	1:A:405:LEU:HD22	2.27	0.65
1:D:57:VAL:HG23	1:D:84:GLN:NE2	2.12	0.64
1:A:3:LYS:O	4:A:440:HOH:O	2.15	0.64
1:B:142:HIS:N	1:B:143:PRO:CD	2.61	0.64
1:D:53:LEU:HG	1:D:130:ASP:HB2	1.78	0.64
1:C:275:THR:HG21	2:C:432:NAD:C8A	2.27	0.64
1:C:220:TYR:CD1	1:C:240:ILE:HD13	2.33	0.64
1:C:334:ARG:HD3	1:C:334:ARG:N	2.12	0.64
1:A:275:THR:O	1:A:304:GLU:OE2	2.16	0.64
1:B:101:TRP:NE1	1:B:104:GLU:HB3	2.13	0.64
1:B:105:THR:OG1	1:B:108:GLU:HG3	1.97	0.64
1:B:275:THR:HG22	1:B:276:GLY:H	1.63	0.64
1:A:300:HIS:HA	1:A:343:LEU:HD11	1.81	0.63
1:D:301:PHE:C	1:D:303:VAL:H	2.06	0.63
1:C:126:MET:HE2	1:C:372:TRP:CB	2.26	0.63
1:A:247:ASN:HA	1:A:250:GLN:NE2	2.10	0.63
1:B:298:ILE:HG12	1:B:298:ILE:O	1.99	0.63
1:C:142:HIS:N	1:C:143:PRO:CD	2.60	0.63
1:B:321:LYS:HB2	1:B:322:PRO:HD2	1.81	0.63
1:A:254:GLU:HG2	4:B:444:HOH:O	1.98	0.63
1:B:420:ILE:HG12	1:B:420:ILE:O	1.99	0.63
1:C:343:LEU:CD2	1:C:346:LEU:HD12	2.27	0.63
1:B:353:PRO:O	1:B:356:VAL:HG13	1.98	0.63
1:C:142:HIS:HB3	1:C:145:LEU:CD1	2.28	0.63
1:B:275:THR:HG21	2:B:432:NAD:C8A	2.29	0.63
1:D:126:MET:HE2	1:D:372:TRP:HB2	1.81	0.63
1:A:190:ASN:N	1:A:190:ASN:HD22	1.95	0.62
1:C:398:LEU:HG	1:C:403:VAL:CG2	2.28	0.62
1:C:37:MET:HE2	1:C:38:TYR:CE2	2.33	0.62
1:B:53:LEU:O	1:B:54:HIS:C	2.41	0.62
1:B:398:LEU:HG	1:B:403:VAL:HG22	1.80	0.62
1:A:308:LYS:H	1:A:308:LYS:HD2	1.63	0.62
1:C:53:LEU:O	1:C:54:HIS:C	2.41	0.62
1:D:37:MET:HE2	1:D:38:TYR:CE2	2.35	0.62
1:D:44:LEU:HB3	1:D:71:ALA:HB2	1.81	0.62
1:A:386:PRO:HG2	1:A:389:LEU:HD12	1.82	0.62
1:C:152:ILE:HD11	1:C:174:VAL:HB	1.82	0.62
1:A:244:ASP:HB3	1:A:247:ASN:HD22	1.65	0.62
1:D:288:GLN:OE1	1:D:288:GLN:HA	2.00	0.62
1:C:72:GLU:HB3	1:C:119:PHE:CE2	2.35	0.62
1:D:142:HIS:N	1:D:143:PRO:CD	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LYS:O	1:D:207:ASP:N	2.33	0.62
1:A:142:HIS:N	1:A:143:PRO:CD	2.61	0.62
1:A:275:THR:HG22	1:A:276:GLY:H	1.63	0.62
1:B:190:ASN:N	1:B:190:ASN:HD22	1.96	0.62
1:D:155:GLU:O	1:D:155:GLU:HG2	1.98	0.62
1:C:142:HIS:HB3	1:C:145:LEU:HD12	1.81	0.62
1:C:321:LYS:HB2	1:C:322:PRO:HD2	1.81	0.62
1:D:110:LEU:O	1:D:114:GLU:HG3	2.00	0.62
1:B:25:GLU:HB3	1:B:32:MET:HE2	1.81	0.61
1:C:28:MET:HB3	1:C:358:SER:HB2	1.82	0.61
1:C:38:TYR:HD1	1:C:43:PRO:HG3	1.65	0.61
1:C:57:VAL:HG23	1:C:84:GLN:NE2	2.15	0.61
1:C:123:PRO:CB	1:C:145:LEU:HD22	2.30	0.61
1:C:301:PHE:C	1:C:303:VAL:H	2.07	0.61
1:C:38:TYR:CD1	1:C:43:PRO:HG3	2.36	0.61
1:D:398:LEU:HG	1:D:403:VAL:CG2	2.30	0.61
1:C:53:LEU:HG	1:C:130:ASP:HB2	1.82	0.61
1:A:243:ILE:HG21	1:B:408:LEU:HD13	1.81	0.61
1:B:124:LEU:H	1:B:124:LEU:HD23	1.65	0.61
1:B:53:LEU:HG	1:B:130:ASP:HB2	1.82	0.61
1:B:334:ARG:HD3	1:B:334:ARG:N	2.14	0.61
1:D:54:HIS:HB3	1:D:82:SER:OG	2.00	0.61
1:D:321:LYS:HB2	1:D:322:PRO:HD2	1.82	0.61
1:D:334:ARG:HD3	1:D:334:ARG:N	2.16	0.61
1:A:321:LYS:HB2	1:A:322:PRO:HD2	1.83	0.61
1:B:126:MET:HE2	1:B:372:TRP:HB2	1.83	0.61
1:B:247:ASN:HA	1:B:250:GLN:NE2	2.16	0.61
1:C:188:PHE:CE1	1:D:249:LEU:HD21	2.36	0.61
1:D:299:GLY:O	2:D:432:NAD:H2N	2.01	0.61
1:B:126:MET:HE1	1:B:371:LEU:HB3	1.83	0.61
1:A:53:LEU:HG	1:A:130:ASP:HB2	1.81	0.61
1:A:247:ASN:HD21	1:B:425:LYS:CE	2.10	0.61
1:B:301:PHE:C	1:B:303:VAL:H	2.09	0.61
1:C:142:HIS:N	1:C:143:PRO:HD3	2.15	0.61
1:D:105:THR:OG1	1:D:108:GLU:HG3	2.00	0.60
1:D:240:ILE:O	1:D:258:VAL:HA	2.00	0.60
1:C:54:HIS:HB3	1:C:82:SER:OG	2.01	0.60
1:B:343:LEU:CD2	1:B:346:LEU:HD12	2.30	0.60
1:D:298:ILE:HG12	1:D:298:ILE:O	2.01	0.60
1:B:57:VAL:HG23	1:B:84:GLN:HE22	1.67	0.60
1:B:166:MET:HA	1:B:171:ILE:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:ND2	1:B:360:SER:HB2	2.16	0.60
1:A:321:LYS:HB2	1:A:322:PRO:CD	2.31	0.60
1:D:275:THR:O	1:D:304:GLU:OE2	2.19	0.60
1:A:203:LYS:O	1:A:207:ASP:N	2.34	0.60
1:B:17:GLY:HA2	1:B:86:HIS:HD2	1.67	0.60
1:B:144:GLN:H	1:B:144:GLN:CD	2.10	0.60
1:C:130:ASP:O	1:C:156:THR:HG21	2.01	0.60
1:D:190:ASN:HD22	1:D:190:ASN:N	1.98	0.60
1:B:200:ASP:O	1:B:204:ARG:HG3	2.02	0.59
1:A:55:MET:HB3	1:A:83:THR:HG23	1.84	0.59
1:B:162:ASN:O	1:B:166:MET:HG3	2.03	0.59
1:B:393:VAL:O	1:B:397:HIS:CD2	2.55	0.59
1:C:398:LEU:CD2	1:C:405:LEU:HD22	2.33	0.59
1:C:127:ILE:CG2	1:C:134:LEU:HD12	2.28	0.59
1:C:139:HIS:CE1	1:C:146:LEU:HD11	2.37	0.59
1:A:398:LEU:HG	1:A:403:VAL:HG22	1.83	0.59
1:B:55:MET:HE1	1:B:63:ILE:CD1	2.32	0.59
1:C:284:ARG:HD2	4:C:440:HOH:O	2.02	0.59
1:D:308:LYS:H	1:D:308:LYS:HD2	1.67	0.59
1:C:178:ASN:HD22	1:C:384:PHE:HE1	1.51	0.59
1:D:42:LYS:N	1:D:43:PRO:CD	2.65	0.59
1:D:393:VAL:O	1:D:397:HIS:HD2	1.85	0.59
1:C:203:LYS:O	1:C:207:ASP:N	2.35	0.59
1:D:321:LYS:HB2	1:D:322:PRO:CD	2.32	0.59
1:B:308:LYS:HD2	1:B:308:LYS:N	2.18	0.58
1:C:244:ASP:CB	1:C:247:ASN:HD22	2.15	0.58
1:A:403:VAL:HB	1:B:258:VAL:HB	1.84	0.58
1:B:389:LEU:O	1:B:392:ALA:HB3	2.02	0.58
1:B:321:LYS:HB2	1:B:322:PRO:CD	2.32	0.58
1:A:27:GLU:C	1:A:29:PRO:HD3	2.29	0.58
1:C:275:THR:HB	1:C:277:CYS:H	1.68	0.58
1:D:53:LEU:O	1:D:54:HIS:C	2.46	0.58
1:A:123:PRO:CB	1:A:145:LEU:HD22	2.32	0.58
1:A:126:MET:HE2	1:A:372:TRP:CB	2.31	0.58
1:B:299:GLY:O	2:B:432:NAD:H2N	2.04	0.58
1:C:245:PRO:HG2	1:D:391:GLU:HB3	1.86	0.58
1:C:249:LEU:HD21	1:D:188:PHE:CE1	2.39	0.58
1:D:300:HIS:HA	1:D:343:LEU:HD11	1.84	0.58
1:B:136:ASN:HD21	1:B:162:ASN:ND2	1.92	0.58
1:B:240:ILE:O	1:B:258:VAL:HA	2.03	0.58
1:C:42:LYS:N	1:C:43:PRO:CD	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:MET:HE1	1:C:371:LEU:HB3	1.86	0.58
1:C:218:ALA:HA	1:C:241:THR:OG1	2.03	0.58
1:D:25:GLU:HB3	1:D:32:MET:HE2	1.86	0.58
1:A:334:ARG:HD3	1:A:334:ARG:N	2.18	0.57
1:C:300:HIS:HA	1:C:343:LEU:HD11	1.86	0.57
1:A:320:ILE:HG22	1:A:321:LYS:HG2	1.85	0.57
1:B:52:CYS:HA	1:B:76:SER:O	2.04	0.57
1:D:275:THR:HG21	2:D:432:NAD:C8A	2.34	0.57
1:B:10:ASP:HB3	1:B:13:LEU:HD23	1.85	0.57
1:B:75:TRP:CH2	1:B:128:LEU:HD13	2.36	0.57
1:B:277:CYS:O	1:B:304:GLU:HG2	2.04	0.57
1:C:430:ARG:HD3	1:D:430:ARG:HA	1.87	0.57
1:B:44:LEU:HB3	1:B:71:ALA:HB2	1.86	0.57
1:B:160:VAL:O	1:B:163:LEU:HB2	2.05	0.57
1:C:162:ASN:O	1:C:166:MET:HG3	2.04	0.57
1:C:328:LEU:HD12	1:C:329:LEU:N	2.19	0.57
1:B:101:TRP:HD1	1:B:102:LYS:O	1.86	0.57
1:D:281:ILE:C	1:D:282:LEU:HD13	2.30	0.57
1:A:382:VAL:O	1:A:382:VAL:HG13	2.03	0.57
1:C:283:GLY:O	1:C:287:GLU:HG3	2.04	0.57
1:C:72:GLU:HB3	1:C:119:PHE:HE2	1.68	0.57
1:D:48:ARG:HB2	1:D:125:ASN:ND2	2.18	0.57
1:D:195:ARG:HG3	1:D:226:GLY:O	2.05	0.57
1:D:283:GLY:O	1:D:287:GLU:HG3	2.05	0.57
1:A:299:GLY:O	2:A:432:NAD:H2N	2.05	0.57
1:A:337:LEU:C	1:A:337:LEU:HD13	2.30	0.57
1:D:13:LEU:HB3	1:D:86:HIS:HA	1.87	0.57
1:D:178:ASN:HD22	1:D:384:PHE:HE1	1.52	0.57
1:C:10:ASP:HB3	1:C:13:LEU:HD23	1.86	0.56
1:B:130:ASP:C	1:B:156:THR:HG21	2.30	0.56
1:D:134:LEU:O	1:D:138:ILE:HG13	2.05	0.56
1:B:37:MET:HE2	1:B:38:TYR:CE2	2.40	0.56
1:B:178:ASN:HD22	1:B:384:PHE:HE1	1.53	0.56
1:B:196:GLU:HG3	1:D:209:MET:HE2	1.88	0.56
1:A:10:ASP:HB3	1:A:13:LEU:HD23	1.87	0.56
1:A:57:VAL:HG23	1:A:84:GLN:NE2	2.20	0.56
1:C:321:LYS:HB2	1:C:322:PRO:CD	2.35	0.56
1:D:389:LEU:O	1:D:392:ALA:HB3	2.05	0.56
1:C:160:VAL:O	1:C:163:LEU:HB2	2.05	0.56
1:B:279:ASP:HA	1:B:282:LEU:HD11	1.88	0.56
1:A:126:MET:HE1	1:A:371:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:MET:HA	1:A:171:ILE:HD12	1.88	0.56
1:B:337:LEU:HD13	1:B:337:LEU:C	2.31	0.56
1:C:155:GLU:O	1:C:155:GLU:HG2	2.05	0.56
1:C:240:ILE:O	1:C:258:VAL:HA	2.05	0.56
1:A:164:TYR:CE1	1:A:382:VAL:HG11	2.40	0.56
1:A:276:GLY:O	1:B:415:TYR:HE2	1.88	0.56
1:B:298:ILE:O	1:B:298:ILE:CG1	2.52	0.56
1:C:25:GLU:HB3	1:C:32:MET:HE2	1.87	0.56
1:B:220:TYR:CD1	1:B:240:ILE:HD13	2.41	0.56
1:C:308:LYS:HD2	1:C:308:LYS:N	2.21	0.56
1:D:101:TRP:NE1	1:D:104:GLU:HB3	2.21	0.56
1:D:307:VAL:O	1:D:310:LEU:HB2	2.05	0.56
1:B:139:HIS:CE1	1:B:146:LEU:HD11	2.42	0.55
1:D:398:LEU:HG	1:D:403:VAL:HG22	1.87	0.55
1:A:53:LEU:O	1:A:54:HIS:C	2.48	0.55
1:B:308:LYS:H	1:B:308:LYS:CD	2.15	0.55
1:C:110:LEU:O	1:C:110:LEU:HD22	2.06	0.55
1:C:353:PRO:HD2	1:C:356:VAL:CG1	2.32	0.55
1:C:373:THR:HG22	1:C:374:HIS:CE1	2.42	0.55
1:D:398:LEU:CD2	1:D:405:LEU:HD22	2.37	0.55
1:C:27:GLU:C	1:C:29:PRO:HD3	2.32	0.55
1:D:123:PRO:CB	1:D:145:LEU:HD22	2.36	0.55
1:A:54:HIS:HB3	1:A:82:SER:OG	2.06	0.55
1:C:188:PHE:HE1	1:D:249:LEU:HD21	1.72	0.55
1:B:142:HIS:CB	1:B:145:LEU:HD12	2.34	0.55
1:B:349:ALA:O	1:B:350:MET:HE2	2.07	0.55
1:C:44:LEU:HB3	1:C:71:ALA:HB2	1.88	0.55
1:C:113:ILE:HG23	1:C:134:LEU:HD23	1.89	0.55
1:D:249:LEU:O	1:D:253:MET:HG2	2.07	0.55
1:A:195:ARG:HG3	1:A:226:GLY:O	2.07	0.55
1:D:353:PRO:O	1:D:356:VAL:CG1	2.54	0.55
1:A:160:VAL:O	1:A:163:LEU:HB2	2.07	0.55
1:D:60:ALA:CA	1:D:91:ILE:HD11	2.37	0.55
1:B:38:TYR:CD1	1:B:43:PRO:HG3	2.41	0.55
1:B:198:LEU:HD22	1:B:227:CYS:HB3	1.88	0.55
1:B:209:MET:HA	1:D:196:GLU:OE1	2.07	0.55
1:B:407:LYS:CD	1:B:420:ILE:HD11	2.36	0.55
1:C:307:VAL:O	1:C:310:LEU:HB2	2.06	0.55
1:A:101:TRP:NE1	1:A:104:GLU:HB3	2.22	0.54
1:B:301:PHE:HB2	1:B:303:VAL:HG22	1.88	0.54
1:D:3:LYS:HD2	1:D:3:LYS:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:N	1:B:143:PRO:HD3	2.21	0.54
1:B:155:GLU:O	1:B:155:GLU:HG2	2.06	0.54
1:A:42:LYS:N	1:A:43:PRO:CD	2.70	0.54
1:A:307:VAL:O	1:A:310:LEU:HB2	2.07	0.54
1:C:308:LYS:H	1:C:308:LYS:CD	2.16	0.54
1:C:408:LEU:HD13	1:D:243:ILE:HG21	1.87	0.54
1:D:38:TYR:CD1	1:D:43:PRO:HG3	2.42	0.54
1:B:124:LEU:HD23	1:B:124:LEU:N	2.21	0.54
1:C:63:ILE:HD12	1:C:91:ILE:HD13	1.90	0.54
1:C:301:PHE:HB2	1:C:303:VAL:HG22	1.90	0.54
1:D:27:GLU:C	1:D:29:PRO:HD3	2.32	0.54
1:B:398:LEU:HG	1:B:403:VAL:HG21	1.90	0.54
1:C:249:LEU:HD21	1:D:188:PHE:HE1	1.73	0.54
1:A:142:HIS:N	1:A:143:PRO:HD3	2.21	0.54
1:A:277:CYS:HB3	1:A:280:ILE:HD11	1.90	0.54
1:A:374:HIS:N	1:A:375:PRO:CD	2.70	0.54
1:A:409:THR:O	1:A:410:GLU:C	2.51	0.54
1:B:369:ILE:O	1:B:373:THR:HB	2.08	0.54
1:C:299:GLY:O	2:C:432:NAD:H2N	2.09	0.54
1:D:28:MET:HA	1:D:358:SER:HB2	1.90	0.54
1:A:155:GLU:O	1:A:155:GLU:HG2	2.08	0.53
1:B:358:SER:OG	1:B:397:HIS:HE1	1.91	0.53
1:A:224:GLY:HA2	1:A:274:THR:HG21	1.90	0.53
1:C:398:LEU:HG	1:C:403:VAL:HG22	1.90	0.53
1:D:386:PRO:HG2	1:D:389:LEU:HD12	1.90	0.53
1:A:44:LEU:HB3	1:A:71:ALA:HB2	1.89	0.53
1:A:277:CYS:O	1:A:304:GLU:HG2	2.08	0.53
1:C:279:ASP:OD2	1:D:411:LYS:HD3	2.09	0.53
1:D:190:ASN:ND2	2:D:432:NAD:H5N	2.23	0.53
1:D:194:CYS:SG	1:D:223:VAL:HG13	2.48	0.53
1:B:16:TRP:O	1:B:19:LYS:HB2	2.07	0.53
1:B:48:ARG:H	1:B:125:ASN:CG	2.15	0.53
1:C:139:HIS:ND1	1:C:146:LEU:HD11	2.24	0.53
1:B:189:ASP:C	1:B:190:ASN:HD22	2.16	0.53
1:D:52:CYS:HA	1:D:76:SER:O	2.09	0.53
1:D:185:ASN:HB2	1:D:363:ASN:ND2	2.23	0.53
1:A:343:LEU:CD2	1:A:346:LEU:HD12	2.38	0.53
1:A:369:ILE:O	1:A:373:THR:HB	2.08	0.53
1:C:200:ASP:O	1:C:204:ARG:HG3	2.09	0.53
1:A:75:TRP:HH2	1:A:128:LEU:HD13	1.74	0.53
1:A:136:ASN:HD21	1:A:162:ASN:ND2	2.00	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:CB	1:B:145:LEU:HD22	2.38	0.53
1:D:273:THR:OG1	1:D:297:ASN:OD1	2.27	0.53
1:D:277:CYS:O	1:D:304:GLU:HG2	2.09	0.53
1:C:126:MET:CE	1:C:372:TRP:HB2	2.36	0.53
1:C:275:THR:HG22	1:C:276:GLY:H	1.74	0.53
1:D:55:MET:HE1	1:D:63:ILE:CD1	2.39	0.53
1:A:24:ALA:O	1:A:28:MET:HG3	2.09	0.53
1:A:178:ASN:N	1:A:383:HIS:O	2.41	0.53
1:A:275:THR:HG23	2:A:432:NAD:O4B	2.08	0.53
1:A:350:MET:HE2	1:A:350:MET:HA	1.90	0.53
1:C:298:ILE:O	1:C:299:GLY:O	2.27	0.53
1:D:372:TRP:CG	1:D:372:TRP:O	2.61	0.53
1:A:52:CYS:HA	1:A:76:SER:O	2.09	0.52
1:B:288:GLN:OE1	1:B:288:GLN:HA	2.09	0.52
1:B:350:MET:HE2	1:B:350:MET:HA	1.91	0.52
1:D:349:ALA:O	1:D:350:MET:HE2	2.09	0.52
1:A:298:ILE:HG12	1:A:298:ILE:O	2.10	0.52
1:C:281:ILE:C	1:C:282:LEU:HD13	2.34	0.52
1:D:38:TYR:HD1	1:D:43:PRO:HG3	1.74	0.52
1:D:425:LYS:HD3	1:D:429:TYR:CE2	2.45	0.52
1:C:179:VAL:HG13	1:C:363:ASN:HB3	1.90	0.52
1:A:353:PRO:HD2	1:A:356:VAL:CG1	2.33	0.52
1:C:75:TRP:HH2	1:C:128:LEU:HD13	1.75	0.52
1:D:130:ASP:O	1:D:156:THR:HG21	2.10	0.52
1:C:279:ASP:HA	1:C:282:LEU:HD11	1.90	0.52
1:A:313:ASN:N	1:A:313:ASN:HD22	2.07	0.52
1:B:10:ASP:OD1	1:B:12:GLY:N	2.42	0.52
1:C:144:GLN:CD	1:C:144:GLN:H	2.16	0.52
1:C:320:ILE:HG22	1:C:321:LYS:HG2	1.91	0.52
1:D:57:VAL:HG23	1:D:84:GLN:HE22	1.74	0.52
1:A:3:LYS:N	1:A:3:LYS:HD2	2.25	0.52
1:A:38:TYR:CD1	1:A:43:PRO:HG3	2.44	0.52
1:A:212:GLY:HA2	1:D:252:ALA:O	2.09	0.52
1:A:283:GLY:O	1:A:287:GLU:HG3	2.09	0.52
1:A:349:ALA:O	1:A:350:MET:HE2	2.10	0.52
1:A:398:LEU:HG	1:A:403:VAL:HG21	1.91	0.52
1:B:190:ASN:ND2	2:B:432:NAD:H5N	2.25	0.52
1:C:224:GLY:HA2	1:C:274:THR:HG21	1.91	0.52
1:C:316:GLU:HG3	1:C:328:LEU:HB3	1.90	0.52
1:A:72:GLU:HB3	1:A:119:PHE:CE2	2.44	0.52
1:B:277:CYS:HB3	1:B:280:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:LYS:HE2	1:D:431:TYR:OH	2.09	0.52
1:A:398:LEU:HD23	1:A:405:LEU:HD22	1.92	0.52
1:C:156:THR:O	1:C:160:VAL:HG23	2.10	0.52
1:C:401:LEU:HD12	1:C:403:VAL:HG13	1.91	0.52
1:A:44:LEU:C	1:A:70:GLY:O	2.53	0.51
1:A:130:ASP:C	1:A:156:THR:HG21	2.35	0.51
1:A:362:THR:HB	1:A:393:VAL:HG13	1.93	0.51
1:B:42:LYS:N	1:B:43:PRO:CD	2.73	0.51
1:C:152:ILE:CD1	1:C:174:VAL:HB	2.41	0.51
1:A:142:HIS:CB	1:A:145:LEU:HD12	2.37	0.51
1:B:27:GLU:C	1:B:29:PRO:HD3	2.35	0.51
1:B:38:TYR:HD1	1:B:43:PRO:HG3	1.73	0.51
1:C:16:TRP:O	1:C:19:LYS:HB2	2.10	0.51
1:C:80:ILE:HG13	1:C:81:PHE:CD2	2.45	0.51
1:A:17:GLY:HA2	1:A:86:HIS:CD2	2.43	0.51
1:D:298:ILE:O	1:D:299:GLY:O	2.29	0.51
1:C:101:TRP:NE1	1:C:104:GLU:HB3	2.24	0.51
1:B:124:LEU:H	1:B:124:LEU:CD2	2.23	0.51
1:B:244:ASP:HB3	1:B:247:ASN:HD22	1.76	0.51
1:C:301:PHE:N	4:C:434:HOH:O	2.36	0.51
1:D:17:GLY:HA2	1:D:86:HIS:HD2	1.76	0.51
1:D:308:LYS:H	1:D:308:LYS:CD	2.22	0.51
1:A:113:ILE:HG23	1:A:134:LEU:HD23	1.91	0.51
1:A:189:ASP:C	1:A:190:ASN:HD22	2.18	0.51
1:C:166:MET:HA	1:C:171:ILE:HD12	1.92	0.51
1:C:323:GLN:CG	1:C:339:ALA:HA	2.35	0.51
1:D:328:LEU:HD12	1:D:329:LEU:N	2.25	0.51
1:A:162:ASN:O	1:A:166:MET:HG3	2.11	0.51
1:A:323:GLN:N	1:A:323:GLN:HE21	2.09	0.51
1:C:337:LEU:HD13	1:C:337:LEU:C	2.36	0.51
1:C:425:LYS:HE2	1:D:247:ASN:ND2	2.26	0.51
1:A:328:LEU:HD12	1:A:329:LEU:N	2.26	0.51
1:B:139:HIS:ND1	1:B:146:LEU:HD11	2.25	0.51
1:C:52:CYS:HA	1:C:76:SER:O	2.11	0.51
1:D:44:LEU:C	1:D:70:GLY:O	2.54	0.51
1:C:288:GLN:HA	1:C:288:GLN:OE1	2.11	0.50
1:C:430:ARG:O	1:C:431:TYR:C	2.54	0.50
1:D:96:ILE:O	1:D:98:VAL:HG23	2.11	0.50
1:D:163:LEU:HD13	1:D:176:ALA:CB	2.41	0.50
1:C:189:ASP:C	1:C:190:ASN:HD22	2.19	0.50
1:C:190:ASN:N	1:C:190:ASN:ND2	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:THR:O	1:D:62:LEU:HB3	2.11	0.50
1:D:101:TRP:HD1	1:D:102:LYS:O	1.93	0.50
1:D:353:PRO:CD	1:D:356:VAL:HG11	2.29	0.50
1:A:124:LEU:N	1:A:124:LEU:HD23	2.27	0.50
1:A:379:PRO:O	1:A:383:HIS:HE1	1.94	0.50
1:B:79:ASN:HB3	1:B:82:SER:OG	2.11	0.50
1:B:349:ALA:C	1:B:350:MET:HE2	2.37	0.50
1:D:275:THR:HG22	1:D:276:GLY:N	2.25	0.50
1:D:401:LEU:HD12	1:D:403:VAL:HG13	1.94	0.50
1:A:155:GLU:HG3	1:A:185:ASN:HD21	1.77	0.50
1:A:301:PHE:HB2	1:A:303:VAL:HG22	1.93	0.50
1:B:127:ILE:CG2	1:B:134:LEU:HD12	2.34	0.50
1:C:275:THR:O	1:C:304:GLU:OE2	2.30	0.50
1:C:374:HIS:N	1:C:375:PRO:CD	2.74	0.50
1:D:370:GLU:OE2	1:D:378:TYR:OH	2.23	0.50
1:A:262:ASP:O	1:A:265:CYS:SG	2.66	0.50
1:A:395:GLU:HA	1:A:398:LEU:HD22	1.92	0.50
1:C:28:MET:CB	1:C:358:SER:HB2	2.41	0.50
1:C:55:MET:HE1	1:C:63:ILE:CD1	2.41	0.50
1:C:185:ASN:HB2	1:C:363:ASN:ND2	2.27	0.50
1:C:276:GLY:O	1:D:415:TYR:HE2	1.93	0.50
1:C:386:PRO:CG	1:C:389:LEU:HD12	2.40	0.50
1:A:196:GLU:HG3	1:C:209:MET:HE2	1.94	0.50
1:B:28:MET:HA	1:B:358:SER:HB2	1.93	0.50
1:C:101:TRP:HD1	1:C:102:LYS:O	1.95	0.50
1:C:398:LEU:HG	1:C:403:VAL:HG21	1.93	0.50
1:D:407:LYS:HD3	1:D:420:ILE:HD11	1.93	0.50
1:B:60:ALA:CA	1:B:91:ILE:HD11	2.40	0.50
1:B:134:LEU:O	1:B:138:ILE:HG13	2.12	0.50
1:B:152:ILE:HD11	1:B:174:VAL:HB	1.93	0.50
1:B:307:VAL:O	1:B:310:LEU:HB2	2.12	0.50
1:C:28:MET:HA	1:C:358:SER:HB2	1.94	0.50
1:C:63:ILE:HD11	1:C:75:TRP:CG	2.47	0.50
1:A:28:MET:HB3	1:A:358:SER:HB2	1.93	0.50
1:C:13:LEU:HB3	1:C:86:HIS:HA	1.93	0.50
1:C:164:TYR:CE1	1:C:382:VAL:HG11	2.47	0.50
1:C:195:ARG:HG3	1:C:226:GLY:O	2.12	0.50
1:D:2:ASP:C	1:D:3:LYS:HD2	2.37	0.50
1:D:281:ILE:HA	1:D:285:HIS:ND1	2.27	0.50
1:D:419:PRO:HB2	1:D:422:GLY:H	1.76	0.50
1:A:190:ASN:ND2	2:A:432:NAD:H5N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LYS:HB2	1:B:165:LYS:NZ	2.27	0.49
1:C:275:THR:HG23	2:C:432:NAD:O4B	2.11	0.49
1:D:113:ILE:HG23	1:D:134:LEU:HD23	1.94	0.49
1:D:279:ASP:HA	1:D:282:LEU:HD11	1.93	0.49
1:A:298:ILE:O	1:A:299:GLY:O	2.28	0.49
1:B:68:ALA:C	1:B:70:GLY:H	2.19	0.49
1:B:208:VAL:HG22	1:B:209:MET:N	2.27	0.49
1:B:398:LEU:CD2	1:B:405:LEU:HD22	2.43	0.49
1:C:138:ILE:O	1:C:139:HIS:C	2.55	0.49
1:C:273:THR:OG1	1:C:297:ASN:HB2	2.11	0.49
1:C:403:VAL:HB	1:D:258:VAL:HB	1.94	0.49
1:A:164:TYR:CD1	1:A:382:VAL:HG11	2.48	0.49
1:A:323:GLN:CG	1:A:339:ALA:HA	2.36	0.49
1:B:224:GLY:HA2	1:B:274:THR:HG21	1.94	0.49
1:C:3:LYS:N	1:C:3:LYS:HD2	2.28	0.49
1:D:278:VAL:HG12	1:D:303:VAL:HB	1.93	0.49
1:D:407:LYS:HE3	1:D:408:LEU:O	2.13	0.49
1:A:258:VAL:HB	1:B:403:VAL:HB	1.94	0.49
1:A:340:GLU:HB3	1:A:342:ARG:NH2	2.28	0.49
1:A:429:TYR:HD2	1:A:431:TYR:CE1	2.30	0.49
1:D:337:LEU:C	1:D:337:LEU:HD13	2.37	0.49
1:D:407:LYS:CD	1:D:420:ILE:HD11	2.43	0.49
1:B:275:THR:O	1:B:304:GLU:OE2	2.30	0.49
1:B:382:VAL:HG13	1:B:382:VAL:O	2.11	0.49
1:C:32:MET:O	1:C:36:GLU:HG3	2.12	0.49
1:D:16:TRP:O	1:D:19:LYS:HB2	2.12	0.49
1:C:185:ASN:ND2	1:C:360:SER:HB2	2.27	0.49
1:A:101:TRP:HD1	1:A:102:LYS:O	1.96	0.49
1:B:47:ALA:HB2	1:B:372:TRP:CE2	2.48	0.49
1:B:96:ILE:O	1:B:98:VAL:HG23	2.13	0.49
1:B:185:ASN:HB2	1:B:363:ASN:ND2	2.28	0.49
1:D:369:ILE:O	1:D:373:THR:HB	2.12	0.49
1:D:425:LYS:HD3	1:D:429:TYR:CD2	2.47	0.49
1:B:249:LEU:O	1:B:253:MET:HG2	2.14	0.48
1:B:409:THR:O	1:B:410:GLU:C	2.56	0.48
1:B:316:GLU:HG3	1:B:328:LEU:HB3	1.95	0.48
1:C:164:TYR:CD1	1:C:382:VAL:HG11	2.48	0.48
1:D:174:VAL:CG1	1:D:175:PRO:HD2	2.43	0.48
1:A:17:GLY:HA3	1:A:86:HIS:O	2.13	0.48
1:A:301:PHE:HB3	1:A:303:VAL:HG13	1.95	0.48
1:C:17:GLY:HA2	1:C:86:HIS:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:MET:HB3	1:D:358:SER:HB2	1.93	0.48
1:D:126:MET:HE1	1:D:371:LEU:HB3	1.94	0.48
1:D:183:VAL:HG21	1:D:431:TYR:CE1	2.48	0.48
1:D:306:ASP:CG	1:D:309:TRP:HB2	2.38	0.48
1:A:275:THR:HB	1:A:277:CYS:H	1.78	0.48
1:B:13:LEU:HB3	1:B:86:HIS:HA	1.95	0.48
1:A:48:ARG:NH1	1:A:123:PRO:O	2.45	0.48
1:B:113:ILE:HG23	1:B:134:LEU:HD23	1.94	0.48
1:C:249:LEU:CD2	1:D:188:PHE:HE1	2.26	0.48
1:C:292:ASP:OD1	1:C:336:ILE:CD1	2.58	0.48
1:D:72:GLU:HB3	1:D:119:PHE:CE2	2.49	0.48
1:D:124:LEU:N	1:D:124:LEU:HD23	2.29	0.48
1:D:127:ILE:CG2	1:D:134:LEU:HD12	2.33	0.48
1:D:220:TYR:CZ	1:D:225:LYS:HG2	2.48	0.48
1:D:374:HIS:N	1:D:375:PRO:CD	2.76	0.48
1:D:393:VAL:O	1:D:397:HIS:CD2	2.67	0.48
1:B:196:GLU:HG3	1:D:209:MET:CE	2.43	0.48
1:C:28:MET:HE1	1:C:58:GLU:HB3	1.95	0.48
1:C:242:GLU:O	1:D:405:LEU:HD12	2.14	0.48
1:A:152:ILE:HD11	1:A:174:VAL:HB	1.96	0.48
1:C:181:ASP:OD1	1:D:428:HIS:CE1	2.67	0.48
1:D:308:LYS:HD2	1:D:308:LYS:N	2.28	0.48
1:A:178:ASN:HD22	1:A:384:PHE:HE1	1.59	0.47
1:B:379:PRO:O	1:B:383:HIS:HE1	1.97	0.47
1:C:27:GLU:O	1:C:29:PRO:HD3	2.14	0.47
1:C:57:VAL:HG23	1:C:84:GLN:HE22	1.78	0.47
1:B:27:GLU:O	1:B:355:PHE:HA	2.14	0.47
1:C:206:THR:OG1	1:C:208:VAL:HG12	2.14	0.47
1:A:13:LEU:HB3	1:A:86:HIS:HA	1.97	0.47
1:A:139:HIS:CE1	1:A:146:LEU:HD11	2.49	0.47
1:A:281:ILE:C	1:A:282:LEU:HD13	2.39	0.47
1:A:292:ASP:OD1	1:A:336:ILE:CD1	2.58	0.47
1:D:298:ILE:O	1:D:298:ILE:CG1	2.61	0.47
1:A:174:VAL:CG1	1:A:175:PRO:HD2	2.43	0.47
1:B:419:PRO:HB2	1:B:422:GLY:H	1.79	0.47
1:C:243:ILE:HG21	1:D:408:LEU:HD13	1.96	0.47
1:C:410:GLU:O	1:C:414:GLN:HB2	2.15	0.47
1:D:241:THR:HG22	1:D:259:THR:O	2.15	0.47
1:B:55:MET:HE1	1:B:63:ILE:HD11	1.97	0.47
1:B:164:TYR:CE1	1:B:382:VAL:HG11	2.50	0.47
1:B:275:THR:HB	1:B:277:CYS:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ASN:O	1:B:349:ALA:HB3	2.15	0.47
1:B:374:HIS:N	1:B:375:PRO:CD	2.77	0.47
1:C:55:MET:HE1	1:C:63:ILE:HD11	1.97	0.47
1:C:393:VAL:O	1:C:397:HIS:HD2	1.98	0.47
1:A:420:ILE:O	1:A:420:ILE:HG12	2.15	0.47
1:B:44:LEU:C	1:B:70:GLY:O	2.57	0.46
1:C:48:ARG:H	1:C:125:ASN:CG	2.23	0.46
1:C:395:GLU:HA	1:C:398:LEU:HD22	1.96	0.46
1:C:415:TYR:HE2	1:D:276:GLY:O	1.98	0.46
1:D:156:THR:O	1:D:160:VAL:HG23	2.15	0.46
1:A:145:LEU:H	1:A:145:LEU:HG	1.45	0.46
1:B:143:PRO:CA	1:B:146:LEU:HD23	2.37	0.46
1:B:212:GLY:HA2	1:C:252:ALA:O	2.15	0.46
1:D:349:ALA:C	1:D:350:MET:HE2	2.41	0.46
1:D:178:ASN:N	1:D:383:HIS:O	2.44	0.46
1:D:189:ASP:C	1:D:190:ASN:HD22	2.23	0.46
1:A:10:ASP:HB3	1:A:13:LEU:CD2	2.46	0.46
1:A:37:MET:HE2	1:A:38:TYR:CE2	2.51	0.46
1:A:208:VAL:HG22	1:A:209:MET:N	2.30	0.46
1:B:209:MET:HG3	1:D:196:GLU:OE1	2.16	0.46
1:C:136:ASN:HD21	1:C:162:ASN:ND2	2.04	0.46
1:A:279:ASP:HA	1:A:282:LEU:HD11	1.97	0.46
1:A:301:PHE:C	1:A:303:VAL:N	2.68	0.46
1:C:372:TRP:O	1:C:372:TRP:CG	2.68	0.46
1:D:10:ASP:HB3	1:D:13:LEU:CD2	2.43	0.46
1:A:218:ALA:HA	1:A:241:THR:OG1	2.15	0.46
1:B:63:ILE:HD11	1:B:75:TRP:CG	2.50	0.46
1:A:72:GLU:HB3	1:A:119:PHE:HE2	1.81	0.46
1:A:139:HIS:ND1	1:A:146:LEU:HD11	2.31	0.46
1:A:144:GLN:CD	1:A:144:GLN:H	2.23	0.46
1:A:196:GLU:HG3	1:C:209:MET:CE	2.46	0.46
1:B:373:THR:HG22	1:B:374:HIS:CE1	2.51	0.46
1:D:334:ARG:HG2	1:D:334:ARG:HH11	1.81	0.46
1:D:407:LYS:HE2	1:D:407:LYS:HB3	1.58	0.46
1:A:387:LYS:O	1:A:391:GLU:HG3	2.15	0.46
1:D:167:MET:HB2	1:D:172:LEU:HD22	1.98	0.46
1:D:316:GLU:HG3	1:D:328:LEU:HB3	1.98	0.46
1:C:48:ARG:NH1	1:C:123:PRO:O	2.49	0.46
1:C:174:VAL:CG1	1:C:175:PRO:HD2	2.45	0.46
1:C:409:THR:O	1:C:410:GLU:C	2.59	0.46
1:D:17:GLY:HA2	1:D:86:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:PHE:C	1:D:303:VAL:N	2.74	0.46
1:A:164:TYR:CE1	1:A:382:VAL:CG1	2.99	0.46
1:B:407:LYS:HD3	1:B:420:ILE:HD11	1.97	0.46
1:D:21:LEU:N	1:D:21:LEU:HD23	2.31	0.46
1:D:53:LEU:HG	1:D:130:ASP:CB	2.45	0.46
1:D:55:MET:HE1	1:D:63:ILE:HD11	1.97	0.46
1:D:60:ALA:CB	1:D:91:ILE:HD11	2.46	0.46
1:A:120:LYS:HD2	1:A:121:ASP:CG	2.42	0.45
1:B:220:TYR:CZ	1:B:225:LYS:HG2	2.51	0.45
1:B:387:LYS:HG2	1:B:423:PRO:HB3	1.97	0.45
1:C:48:ARG:HG2	1:C:119:PHE:CD2	2.52	0.45
1:C:130:ASP:C	1:C:156:THR:HG21	2.41	0.45
1:D:152:ILE:HD11	1:D:174:VAL:HB	1.98	0.45
1:A:288:GLN:OE1	1:A:288:GLN:HA	2.17	0.45
1:B:10:ASP:HB3	1:B:13:LEU:CD2	2.46	0.45
1:B:59:THR:O	1:B:62:LEU:HB3	2.16	0.45
1:B:74:ARG:HG3	1:B:97:PRO:HB2	1.98	0.45
1:C:298:ILE:O	1:C:298:ILE:HG12	2.15	0.45
1:D:224:GLY:HA2	1:D:274:THR:HG21	1.97	0.45
1:A:38:TYR:HD1	1:A:43:PRO:HG3	1.81	0.45
1:A:244:ASP:CB	1:A:247:ASN:HD22	2.28	0.45
1:B:60:ALA:CB	1:B:91:ILE:HD11	2.47	0.45
1:D:46:GLY:O	1:D:372:TRP:CH2	2.69	0.45
1:D:398:LEU:HG	1:D:403:VAL:HG21	1.98	0.45
1:A:393:VAL:O	1:A:397:HIS:CD2	2.66	0.45
1:B:399:GLY:O	1:B:400:LYS:C	2.58	0.45
1:C:44:LEU:C	1:C:70:GLY:O	2.59	0.45
1:C:74:ARG:HG3	1:C:97:PRO:HB2	1.98	0.45
1:C:151:GLY:HA3	1:C:371:LEU:HG	1.98	0.45
1:C:301:PHE:HB3	1:C:303:VAL:HG13	1.99	0.45
1:C:416:LEU:HD11	1:D:277:CYS:SG	2.56	0.45
1:D:329:LEU:C	1:D:331:ASN:H	2.24	0.45
1:A:407:LYS:CD	1:A:420:ILE:HD11	2.46	0.45
1:B:275:THR:HG23	2:B:432:NAD:O4B	2.17	0.45
1:D:275:THR:HG23	2:D:432:NAD:O4B	2.15	0.45
1:D:285:HIS:O	1:D:288:GLN:HB2	2.16	0.45
1:B:136:ASN:O	1:B:137:LEU:C	2.59	0.45
1:B:178:ASN:N	1:B:383:HIS:O	2.46	0.45
1:C:28:MET:HA	1:C:358:SER:CB	2.46	0.45
1:D:318:VAL:HG22	1:D:326:ARG:O	2.17	0.45
1:A:407:LYS:HB3	1:A:407:LYS:HE2	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:NH1	1:B:123:PRO:O	2.49	0.45
1:B:275:THR:HG22	1:B:276:GLY:N	2.31	0.45
1:C:83:THR:HG22	1:C:84:GLN:N	2.31	0.45
1:C:164:TYR:CE1	1:C:382:VAL:CG1	3.00	0.45
1:D:244:ASP:OD2	1:D:244:ASP:C	2.60	0.45
1:A:124:LEU:HD23	1:A:124:LEU:H	1.81	0.45
1:A:134:LEU:O	1:A:138:ILE:HG13	2.17	0.45
1:A:136:ASN:O	1:A:137:LEU:C	2.59	0.45
1:A:374:HIS:O	1:A:377:LYS:HB2	2.16	0.45
1:B:17:GLY:HA2	1:B:86:HIS:CD2	2.48	0.45
1:B:79:ASN:HB3	1:B:82:SER:HG	1.81	0.45
1:D:320:ILE:HG22	1:D:321:LYS:HG2	1.98	0.45
1:D:350:MET:HE2	1:D:350:MET:HA	1.99	0.45
1:A:137:LEU:HD12	1:A:141:LYS:HD2	1.98	0.45
1:A:163:LEU:HD13	1:A:176:ALA:CB	2.47	0.45
1:A:408:LEU:HD13	1:B:243:ILE:HG21	1.99	0.45
1:B:156:THR:O	1:B:160:VAL:HG23	2.16	0.45
1:B:328:LEU:HD12	1:B:329:LEU:N	2.31	0.45
1:C:313:ASN:N	1:C:313:ASN:HD22	2.15	0.45
1:A:25:GLU:HB3	1:A:32:MET:HE2	1.99	0.45
1:A:240:ILE:O	1:A:258:VAL:HA	2.16	0.45
1:A:242:GLU:O	1:B:406:THR:HB	2.17	0.45
1:B:21:LEU:N	1:B:21:LEU:HD23	2.32	0.45
1:B:72:GLU:HB3	1:B:119:PHE:CE2	2.51	0.45
1:B:195:ARG:HG3	1:B:226:GLY:O	2.17	0.45
1:C:329:LEU:C	1:C:331:ASN:H	2.24	0.45
1:A:308:LYS:HD2	1:A:308:LYS:N	2.31	0.44
1:D:174:VAL:HG12	1:D:175:PRO:HD2	2.00	0.44
1:A:190:ASN:N	1:A:190:ASN:ND2	2.62	0.44
1:B:24:ALA:O	1:B:28:MET:HG3	2.17	0.44
1:D:218:ALA:HA	1:D:241:THR:OG1	2.17	0.44
1:D:409:THR:O	1:D:410:GLU:C	2.60	0.44
1:A:63:ILE:HG12	1:A:75:TRP:CE3	2.53	0.44
1:A:152:ILE:O	1:A:176:ALA:HA	2.17	0.44
1:B:127:ILE:HD11	1:B:138:ILE:HD12	1.99	0.44
1:C:111:TRP:O	1:C:115:GLN:HG2	2.18	0.44
1:C:194:CYS:SG	1:C:223:VAL:HG13	2.57	0.44
1:C:278:VAL:HG13	1:D:415:TYR:CE2	2.52	0.44
1:A:84:GLN:O	1:A:87:ALA:HB3	2.18	0.44
1:A:389:LEU:O	1:A:393:VAL:HG23	2.18	0.44
1:C:74:ARG:HB3	1:C:116:THR:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:TRP:HH2	1:D:128:LEU:HD13	1.81	0.44
1:A:198:LEU:HD22	1:A:227:CYS:HB3	2.00	0.44
1:A:374:HIS:N	1:A:375:PRO:HD2	2.32	0.44
1:B:218:ALA:HA	1:B:241:THR:OG1	2.17	0.44
1:C:21:LEU:HD23	1:C:21:LEU:N	2.31	0.44
1:D:63:ILE:HD11	1:D:75:TRP:CG	2.52	0.44
1:D:189:ASP:O	1:D:189:ASP:OD2	2.36	0.44
1:A:54:HIS:HA	1:A:77:SER:OG	2.18	0.44
1:A:209:MET:HG3	1:C:196:GLU:OE1	2.17	0.44
1:A:386:PRO:CG	1:A:389:LEU:HD12	2.46	0.44
1:B:27:GLU:OE2	1:B:400:LYS:HE2	2.18	0.44
1:C:184:THR:HB	1:C:359:ASN:HD22	1.83	0.44
1:C:278:VAL:HG12	1:C:303:VAL:HB	2.00	0.44
1:D:425:LYS:HD3	1:D:429:TYR:CZ	2.53	0.44
1:B:79:ASN:OD1	1:B:80:ILE:N	2.51	0.44
1:B:189:ASP:O	1:B:189:ASP:OD2	2.36	0.44
1:C:101:TRP:HZ2	1:C:108:GLU:CD	2.26	0.44
1:A:55:MET:HE1	1:A:63:ILE:CD1	2.48	0.44
1:A:253:MET:HB3	1:A:253:MET:HE3	1.78	0.44
1:A:345:ASN:O	1:A:349:ALA:HB3	2.17	0.44
1:B:46:GLY:O	1:B:372:TRP:CH2	2.71	0.44
1:B:410:GLU:O	1:B:414:GLN:HB2	2.18	0.44
1:C:17:GLY:HA2	1:C:86:HIS:CD2	2.53	0.44
1:C:369:ILE:O	1:C:373:THR:HB	2.17	0.44
1:D:243:ILE:HG13	1:D:244:ASP:N	2.32	0.44
1:D:387:LYS:O	1:D:391:GLU:HG3	2.18	0.44
1:A:5:PRO:O	1:A:97:PRO:HA	2.18	0.44
1:A:91:ILE:HG22	1:A:98:VAL:HG21	2.00	0.44
1:A:373:THR:HG22	1:A:374:HIS:CE1	2.53	0.44
1:B:46:GLY:C	1:B:372:TRP:CZ2	2.96	0.44
1:C:68:ALA:C	1:C:70:GLY:H	2.26	0.44
1:C:243:ILE:HD13	1:D:408:LEU:HD22	2.00	0.44
1:D:142:HIS:N	1:D:143:PRO:HD3	2.32	0.44
1:B:48:ARG:H	1:B:125:ASN:ND2	2.16	0.43
1:B:102:LYS:O	1:B:103:GLY:C	2.60	0.43
1:B:209:MET:HE2	1:D:196:GLU:CG	2.44	0.43
1:C:391:GLU:HB3	1:D:245:PRO:HG2	1.99	0.43
1:D:27:GLU:O	1:D:355:PHE:HA	2.18	0.43
1:D:165:LYS:HB2	1:D:165:LYS:NZ	2.33	0.43
1:A:313:ASN:N	1:A:313:ASN:ND2	2.67	0.43
1:D:275:THR:HB	1:D:277:CYS:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LYS:HE2	1:A:431:TYR:OH	2.17	0.43
1:C:398:LEU:HD23	1:C:405:LEU:HD22	1.98	0.43
1:D:80:ILE:HG13	1:D:81:PHE:CD2	2.53	0.43
1:C:128:LEU:HD21	1:C:364:GLN:HG2	2.00	0.43
1:C:190:ASN:ND2	2:C:432:NAD:H5N	2.34	0.43
1:C:389:LEU:O	1:C:392:ALA:HB3	2.18	0.43
1:A:96:ILE:O	1:A:98:VAL:HG23	2.19	0.43
1:C:220:TYR:CZ	1:C:225:LYS:HG2	2.54	0.43
1:C:373:THR:HG22	1:C:373:THR:O	2.19	0.43
1:C:430:ARG:HA	1:D:430:ARG:HD3	2.00	0.43
1:A:185:ASN:HB2	1:A:363:ASN:ND2	2.34	0.43
1:B:164:TYR:CD1	1:B:382:VAL:HG11	2.53	0.43
1:D:48:ARG:H	1:D:125:ASN:CG	2.24	0.43
1:D:102:LYS:O	1:D:103:GLY:C	2.60	0.43
1:D:136:ASN:ND2	1:D:162:ASN:HD21	2.08	0.43
1:D:336:ILE:HD12	1:D:336:ILE:N	2.33	0.43
1:D:357:MET:HE1	3:D:433:ADN:O2'	2.17	0.43
1:D:142:HIS:HB3	1:D:145:LEU:HD11	2.00	0.43
1:D:299:GLY:HA3	1:D:304:GLU:OE2	2.19	0.43
1:C:259:THR:HA	1:D:404:LYS:HB2	2.01	0.43
1:D:124:LEU:HD23	1:D:124:LEU:H	1.83	0.43
1:A:91:ILE:CG2	1:A:98:VAL:HG21	2.49	0.43
1:D:385:LEU:CD1	1:D:386:PRO:HD2	2.40	0.43
1:A:124:LEU:H	1:A:124:LEU:CD2	2.31	0.43
1:C:349:ALA:C	1:C:350:MET:HE2	2.43	0.43
1:C:393:VAL:O	1:C:397:HIS:CD2	2.71	0.43
1:D:334:ARG:HG2	1:D:334:ARG:NH1	2.33	0.43
1:C:145:LEU:H	1:C:145:LEU:HG	1.51	0.42
1:C:152:ILE:O	1:C:176:ALA:HA	2.18	0.42
1:C:277:CYS:O	1:C:304:GLU:HG2	2.19	0.42
1:D:145:LEU:H	1:D:145:LEU:HG	1.45	0.42
1:D:373:THR:O	1:D:373:THR:HG22	2.18	0.42
1:C:174:VAL:HG12	1:C:175:PRO:HD2	2.00	0.42
1:C:407:LYS:HB3	1:C:407:LYS:HE2	1.46	0.42
1:D:301:PHE:HB2	1:D:303:VAL:HG22	2.01	0.42
1:D:385:LEU:HD12	1:D:385:LEU:HA	1.88	0.42
1:B:174:VAL:CG1	1:B:175:PRO:HD2	2.48	0.42
1:C:10:ASP:HB3	1:C:13:LEU:CD2	2.50	0.42
1:C:74:ARG:HB3	1:C:116:THR:HB	2.01	0.42
1:D:21:LEU:HD23	1:D:57:VAL:HG13	1.99	0.42
1:D:68:ALA:C	1:D:70:GLY:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:O	1:A:144:GLN:C	2.61	0.42
1:B:63:ILE:HD12	1:B:91:ILE:HD13	2.01	0.42
1:B:130:ASP:C	1:B:156:THR:CG2	2.92	0.42
1:B:143:PRO:O	1:B:144:GLN:C	2.61	0.42
1:B:313:ASN:N	1:B:313:ASN:HD22	2.17	0.42
1:C:7:LYS:HD2	1:C:7:LYS:HA	1.79	0.42
1:D:48:ARG:NH1	1:D:123:PRO:O	2.52	0.42
1:D:72:GLU:HB3	1:D:119:PHE:HE2	1.82	0.42
1:A:67:VAL:O	1:A:70:GLY:N	2.51	0.42
1:A:167:MET:HB2	1:A:172:LEU:HD22	2.01	0.42
1:D:28:MET:CB	1:D:358:SER:HB2	2.49	0.42
1:D:73:VAL:CG1	1:D:75:TRP:HE3	2.32	0.42
1:D:184:THR:HB	1:D:359:ASN:HD22	1.84	0.42
1:D:310:LEU:HD13	1:D:327:TYR:CD1	2.55	0.42
1:A:63:ILE:HD11	1:A:75:TRP:CG	2.53	0.42
1:A:63:ILE:HD12	1:A:91:ILE:HD13	2.00	0.42
1:A:298:ILE:O	1:A:298:ILE:CG1	2.68	0.42
1:A:429:TYR:HD2	1:A:431:TYR:CD1	2.37	0.42
1:B:301:PHE:HB3	1:B:303:VAL:HG13	2.01	0.42
1:B:412:GLN:O	1:B:413:ALA:C	2.61	0.42
1:C:388:LYS:HE3	4:C:443:HOH:O	2.19	0.42
1:D:7:LYS:HA	1:D:7:LYS:HD2	1.81	0.42
1:D:177:ILE:O	1:D:177:ILE:HG22	2.19	0.42
1:D:360:SER:HA	1:D:363:ASN:HD22	1.84	0.42
1:A:373:THR:HG22	1:A:373:THR:O	2.18	0.42
1:A:407:LYS:HE3	1:A:408:LEU:O	2.20	0.42
1:D:274:THR:O	2:D:432:NAD:H51N	2.19	0.42
1:D:373:THR:HG22	1:D:374:HIS:CE1	2.55	0.42
1:A:10:ASP:OD1	1:A:12:GLY:N	2.52	0.42
1:A:171:ILE:O	1:A:173:LYS:HG3	2.20	0.42
1:A:310:LEU:HD13	1:A:327:TYR:CD1	2.55	0.42
1:B:279:ASP:CA	1:B:282:LEU:HD11	2.49	0.42
1:B:298:ILE:O	1:B:299:GLY:O	2.36	0.42
1:B:118:HIS:CE1	1:B:123:PRO:HB3	2.55	0.42
1:B:143:PRO:HA	1:B:146:LEU:CD2	2.38	0.42
1:B:282:LEU:HD13	1:B:282:LEU:N	2.34	0.42
1:C:284:ARG:CD	4:C:440:HOH:O	2.66	0.42
1:C:408:LEU:HD12	1:C:408:LEU:HA	1.86	0.42
1:D:55:MET:HB3	1:D:83:THR:HG23	2.01	0.42
1:D:74:ARG:HB3	1:D:116:THR:CB	2.49	0.42
1:D:144:GLN:CD	1:D:144:GLN:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:O	1:A:359:ASN:HB2	2.20	0.42
1:B:53:LEU:HG	1:B:130:ASP:CB	2.48	0.42
1:B:105:THR:O	1:B:108:GLU:N	2.53	0.42
1:B:124:LEU:HD11	1:B:138:ILE:CD1	2.50	0.42
1:C:146:LEU:C	1:C:148:GLY:N	2.78	0.42
1:C:407:LYS:HE3	1:C:408:LEU:O	2.20	0.42
1:D:371:LEU:HD12	1:D:371:LEU:HA	1.78	0.42
1:A:373:THR:C	1:A:375:PRO:HD2	2.45	0.41
1:C:124:LEU:HD23	1:C:124:LEU:N	2.35	0.41
1:C:220:TYR:HB3	1:C:247:ASN:HB3	2.01	0.41
1:D:162:ASN:O	1:D:166:MET:HG3	2.20	0.41
1:D:296:CYS:HB3	1:D:338:LEU:HD12	2.01	0.41
1:A:27:GLU:OE2	1:A:400:LYS:HE2	2.20	0.41
1:A:68:ALA:C	1:A:70:GLY:H	2.28	0.41
1:A:249:LEU:O	1:A:253:MET:HG2	2.20	0.41
1:B:17:GLY:HA3	1:B:86:HIS:O	2.20	0.41
1:B:32:MET:O	1:B:36:GLU:HG3	2.20	0.41
1:B:145:LEU:H	1:B:145:LEU:HG	1.48	0.41
1:C:91:ILE:O	1:C:96:ILE:HB	2.19	0.41
1:C:96:ILE:O	1:C:98:VAL:HG23	2.19	0.41
1:C:153:SER:OG	1:C:368:GLN:NE2	2.53	0.41
1:D:130:ASP:C	1:D:156:THR:HG21	2.45	0.41
1:D:146:LEU:HD13	1:D:146:LEU:HA	1.93	0.41
1:D:208:VAL:HG22	1:D:209:MET:N	2.35	0.41
1:D:301:PHE:HB3	1:D:303:VAL:HG13	2.02	0.41
1:A:75:TRP:CH2	1:A:128:LEU:HD13	2.54	0.41
1:A:424:PHE:O	1:A:425:LYS:HG2	2.20	0.41
1:B:7:LYS:HA	1:B:7:LYS:HD2	1.80	0.41
1:C:350:MET:HE2	1:C:350:MET:HA	2.02	0.41
1:D:13:LEU:HD12	1:D:16:TRP:HE3	1.86	0.41
1:D:150:ARG:HD2	1:D:372:TRP:HA	2.02	0.41
1:D:200:ASP:OD2	1:D:204:ARG:NH2	2.53	0.41
1:A:55:MET:HE1	1:A:63:ILE:HD11	2.02	0.41
1:A:357:MET:HE1	3:A:433:ADN:O2'	2.20	0.41
1:C:249:LEU:O	1:C:250:GLN:C	2.62	0.41
1:D:28:MET:HA	1:D:358:SER:CB	2.50	0.41
1:B:101:TRP:CE2	1:B:104:GLU:HB3	2.55	0.41
1:C:13:LEU:HD12	1:C:16:TRP:CE3	2.55	0.41
1:C:425:LYS:CD	1:C:429:TYR:CE2	3.03	0.41
1:D:13:LEU:HD12	1:D:16:TRP:CE3	2.55	0.41
1:D:190:ASN:N	1:D:190:ASN:ND2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:O	1:B:103:GLY:N	2.54	0.41
1:B:152:ILE:O	1:B:176:ALA:HA	2.20	0.41
1:C:60:ALA:CA	1:C:91:ILE:HD11	2.46	0.41
1:D:48:ARG:HG2	1:D:119:PHE:CD2	2.55	0.41
1:D:134:LEU:O	1:D:134:LEU:HD13	2.21	0.41
1:A:91:ILE:HG22	1:A:98:VAL:CG2	2.50	0.41
1:A:329:LEU:HB2	1:A:331:ASN:OD1	2.19	0.41
1:A:349:ALA:C	1:A:350:MET:HE2	2.45	0.41
1:B:401:LEU:HD12	1:B:403:VAL:HG13	2.03	0.41
1:C:329:LEU:HB2	1:C:331:ASN:OD1	2.21	0.41
1:C:349:ALA:O	1:C:350:MET:HE2	2.20	0.41
1:D:55:MET:SD	1:D:91:ILE:HD12	2.61	0.41
1:D:143:PRO:O	1:D:144:GLN:C	2.63	0.41
1:D:313:ASN:N	1:D:313:ASN:HD22	2.18	0.41
1:D:379:PRO:O	1:D:383:HIS:HE1	2.03	0.41
1:A:142:HIS:HB3	1:A:145:LEU:HD11	2.00	0.41
1:A:278:VAL:HG12	1:A:303:VAL:HB	2.03	0.41
1:C:59:THR:O	1:C:62:LEU:HB3	2.20	0.41
1:C:188:PHE:HE1	1:D:249:LEU:CD2	2.33	0.41
1:D:395:GLU:HA	1:D:398:LEU:HD22	2.02	0.41
1:A:7:LYS:HD2	1:A:7:LYS:HA	1.92	0.41
1:A:160:VAL:HG12	1:A:164:TYR:CE2	2.56	0.41
1:A:200:ASP:O	1:A:204:ARG:HG3	2.21	0.41
1:A:379:PRO:O	1:A:383:HIS:CE1	2.74	0.41
1:B:14:ALA:O	1:B:15:ALA:C	2.63	0.41
1:B:72:GLU:HB3	1:B:119:PHE:HE2	1.86	0.41
1:B:340:GLU:HB3	1:B:342:ARG:NH2	2.36	0.41
1:B:371:LEU:HD12	1:B:371:LEU:HA	1.91	0.41
1:C:108:GLU:O	1:C:111:TRP:HB3	2.21	0.41
1:C:299:GLY:HA3	1:C:304:GLU:OE2	2.21	0.41
1:C:373:THR:O	1:C:373:THR:CG2	2.69	0.41
2:C:432:NAD:H3B	1:D:425:LYS:NZ	2.36	0.41
1:D:63:ILE:HD12	1:D:91:ILE:HD13	2.02	0.41
1:D:165:LYS:O	1:D:166:MET:C	2.63	0.41
1:A:32:MET:O	1:A:36:GLU:HG3	2.21	0.41
1:A:58:GLU:HG2	1:A:354:SER:HA	2.01	0.41
1:A:365:VAL:O	1:A:369:ILE:HG13	2.21	0.41
1:B:3:LYS:N	1:B:3:LYS:HD2	2.36	0.41
1:C:109:TYR:CE2	1:C:113:ILE:HD11	2.56	0.41
1:C:403:VAL:CG2	1:C:403:VAL:O	2.67	0.41
1:A:137:LEU:CD1	1:A:141:LYS:HD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLU:HG3	1:A:328:LEU:HB3	2.03	0.40
1:B:252:ALA:O	1:C:212:GLY:HA2	2.22	0.40
1:B:292:ASP:OD1	1:B:336:ILE:CD1	2.62	0.40
1:B:353:PRO:CD	1:B:356:VAL:HG11	2.33	0.40
1:C:285:HIS:O	1:C:288:GLN:HB2	2.21	0.40
1:C:379:PRO:O	1:C:383:HIS:CE1	2.74	0.40
1:D:17:GLY:HA3	1:D:86:HIS:O	2.22	0.40
1:D:74:ARG:HB3	1:D:116:THR:HB	2.03	0.40
1:A:333:HIS:C	1:A:334:ARG:HD3	2.45	0.40
1:A:353:PRO:O	1:A:356:VAL:CG1	2.65	0.40
1:B:101:TRP:HZ2	1:B:108:GLU:CD	2.29	0.40
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.92	0.40
1:C:5:PRO:O	1:C:97:PRO:HA	2.21	0.40
1:C:73:VAL:CG1	1:C:75:TRP:HE3	2.34	0.40
1:C:183:VAL:HG21	1:C:431:TYR:CE1	2.56	0.40
1:C:399:GLY:O	1:C:400:LYS:C	2.64	0.40
1:A:57:VAL:O	1:A:61:VAL:HG23	2.22	0.40
1:A:281:ILE:HA	1:A:285:HIS:ND1	2.35	0.40
1:B:223:VAL:HG12	1:B:274:THR:HG22	2.04	0.40
1:D:96:ILE:HA	1:D:97:PRO:HD3	1.96	0.40
1:A:5:PRO:O	1:A:6:TYR:HB3	2.22	0.40
1:A:275:THR:HG22	1:A:276:GLY:N	2.33	0.40
1:A:329:LEU:C	1:A:331:ASN:H	2.28	0.40
1:B:74:ARG:NH1	1:B:115:GLN:O	2.54	0.40
1:B:178:ASN:HD21	1:B:181:ASP:CG	2.29	0.40
1:C:367:ALA:O	1:C:371:LEU:HB2	2.21	0.40
1:D:126:MET:HE2	1:D:372:TRP:CB	2.49	0.40
1:A:143:PRO:CA	1:A:146:LEU:HD23	2.40	0.40
1:A:174:VAL:HG12	1:A:175:PRO:HD2	2.04	0.40
1:A:178:ASN:HD21	1:A:181:ASP:CG	2.29	0.40
1:A:209:MET:HA	1:C:196:GLU:OE1	2.22	0.40
1:A:320:ILE:O	1:A:321:LYS:HB3	2.21	0.40
1:A:407:LYS:CE	1:A:420:ILE:HD11	2.52	0.40
1:C:389:LEU:O	1:C:393:VAL:HG23	2.22	0.40
1:D:46:GLY:C	1:D:372:TRP:CZ2	3.00	0.40
1:D:279:ASP:CA	1:D:282:LEU:HD11	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/431 (99%)	378 (88%)	43 (10%)	7 (2%)	7	27
1	B	428/431 (99%)	377 (88%)	45 (10%)	6 (1%)	9	30
1	C	428/431 (99%)	374 (87%)	48 (11%)	6 (1%)	9	30
1	D	428/431 (99%)	370 (86%)	52 (12%)	6 (1%)	9	30
All	All	1712/1724 (99%)	1499 (88%)	188 (11%)	25 (2%)	8	28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLY
1	B	103	GLY
1	B	299	GLY
1	C	299	GLY
1	C	339	ALA
1	D	103	GLY
1	D	299	GLY
1	D	339	ALA
1	A	13	LEU
1	B	339	ALA
1	A	302	ASP
1	A	339	ALA
1	B	13	LEU
1	B	70	GLY
1	B	131	GLY
1	D	70	GLY
1	A	70	GLY
1	C	70	GLY
1	C	131	GLY
1	D	131	GLY
1	A	103	GLY
1	A	410	GLU

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Mol	Chain	Res	Type
1	D	268	GLY
1	C	103	GLY
1	C	315	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/353 (100%)	317 (90%)	36 (10%)	7	23
1	B	353/353 (100%)	312 (88%)	41 (12%)	5	18
1	C	353/353 (100%)	312 (88%)	41 (12%)	5	18
1	D	353/353 (100%)	312 (88%)	41 (12%)	5	18
All	All	1412/1412 (100%)	1253 (89%)	159 (11%)	5	19

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	23	ILE
1	A	33	ARG
1	A	39	SER
1	A	53	LEU
1	A	93	LYS
1	A	120	LYS
1	A	133	ASP
1	A	139	HIS
1	A	144	GLN
1	A	145	LEU
1	A	158	THR
1	A	177	ILE
1	A	190	ASN
1	A	213	LYS
1	A	267	GLU
1	A	275	THR
1	A	282	LEU

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Mol	Chain	Res	Type
1	A	297	ASN
1	A	307	VAL
1	A	308	LYS
1	A	313	ASN
1	A	323	GLN
1	A	328	LEU
1	A	334	ARG
1	A	340	GLU
1	A	356	VAL
1	A	357	MET
1	A	371	LEU
1	A	388	LYS
1	A	398	LEU
1	A	401	LEU
1	A	403	VAL
1	A	407	LYS
1	A	414	GLN
1	A	420	ILE
1	B	3	LYS
1	B	21	LEU
1	B	23	ILE
1	B	33	ARG
1	B	39	SER
1	B	41	SER
1	B	74	ARG
1	B	93	LYS
1	B	110	LEU
1	B	120	LYS
1	B	133	ASP
1	B	139	HIS
1	B	144	GLN
1	B	145	LEU
1	B	158	THR
1	B	165	LYS
1	B	169	ASN
1	B	190	ASN
1	B	199	ILE
1	B	213	LYS
1	B	250	GLN
1	B	267	GLU
1	B	275	THR
1	B	282	LEU

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Mol	Chain	Res	Type
1	B	308	LYS
1	B	313	ASN
1	B	323	GLN
1	B	334	ARG
1	B	340	GLU
1	B	356	VAL
1	B	357	MET
1	B	371	LEU
1	B	387	LYS
1	B	388	LYS
1	B	398	LEU
1	B	401	LEU
1	B	403	VAL
1	B	407	LYS
1	B	408	LEU
1	B	414	GLN
1	B	420	ILE
1	C	3	LYS
1	C	21	LEU
1	C	23	ILE
1	C	33	ARG
1	C	39	SER
1	C	41	SER
1	C	53	LEU
1	C	74	ARG
1	C	93	LYS
1	C	110	LEU
1	C	120	LYS
1	C	133	ASP
1	C	139	HIS
1	C	144	GLN
1	C	145	LEU
1	C	154	GLU
1	C	158	THR
1	C	190	ASN
1	C	213	LYS
1	C	250	GLN
1	C	267	GLU
1	C	275	THR
1	C	282	LEU
1	C	297	ASN
1	C	308	LYS

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Mol	Chain	Res	Type
1	C	312	GLU
1	C	313	ASN
1	C	323	GLN
1	C	334	ARG
1	C	340	GLU
1	C	356	VAL
1	C	357	MET
1	C	371	LEU
1	C	388	LYS
1	C	398	LEU
1	C	401	LEU
1	C	403	VAL
1	C	407	LYS
1	C	408	LEU
1	C	414	GLN
1	C	420	ILE
1	D	3	LYS
1	D	21	LEU
1	D	23	ILE
1	D	33	ARG
1	D	39	SER
1	D	41	SER
1	D	53	LEU
1	D	93	LYS
1	D	120	LYS
1	D	133	ASP
1	D	139	HIS
1	D	144	GLN
1	D	145	LEU
1	D	154	GLU
1	D	158	THR
1	D	165	LYS
1	D	169	ASN
1	D	177	ILE
1	D	190	ASN
1	D	213	LYS
1	D	250	GLN
1	D	267	GLU
1	D	275	THR
1	D	282	LEU
1	D	308	LYS
1	D	312	GLU

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Mol	Chain	Res	Type
1	D	313	ASN
1	D	323	GLN
1	D	334	ARG
1	D	340	GLU
1	D	356	VAL
1	D	357	MET
1	D	371	LEU
1	D	388	LYS
1	D	398	LEU
1	D	401	LEU
1	D	403	VAL
1	D	407	LYS
1	D	408	LEU
1	D	414	GLN
1	D	420	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	84	GLN
1	A	86	HIS
1	A	136	ASN
1	A	190	ASN
1	A	247	ASN
1	A	250	GLN
1	A	269	ASN
1	A	300	HIS
1	A	313	ASN
1	A	323	GLN
1	A	359	ASN
1	A	363	ASN
1	A	368	GLN
1	A	374	HIS
1	A	383	HIS
1	A	397	HIS
1	A	412	GLN
1	B	84	GLN
1	B	86	HIS
1	B	136	ASN
1	B	190	ASN
1	B	247	ASN

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Mol	Chain	Res	Type
1	B	250	GLN
1	B	269	ASN
1	B	300	HIS
1	B	313	ASN
1	B	323	GLN
1	B	359	ASN
1	B	363	ASN
1	B	368	GLN
1	B	374	HIS
1	B	383	HIS
1	B	397	HIS
1	C	26	ASN
1	C	84	GLN
1	C	86	HIS
1	C	136	ASN
1	C	190	ASN
1	C	247	ASN
1	C	250	GLN
1	C	269	ASN
1	C	300	HIS
1	C	313	ASN
1	C	323	GLN
1	C	352	HIS
1	C	363	ASN
1	C	368	GLN
1	C	397	HIS
1	C	412	GLN
1	D	84	GLN
1	D	86	HIS
1	D	136	ASN
1	D	190	ASN
1	D	247	ASN
1	D	250	GLN
1	D	269	ASN
1	D	300	HIS
1	D	313	ASN
1	D	323	GLN
1	D	363	ASN
1	D	368	GLN
1	D	397	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	ADN	B	433	-	21,21,21	1.33	4 (19%)	31,31,31	1.31	3 (9%)
2	NAD	D	432	-	46,48,48	2.67	9 (19%)	64,73,73	1.45	9 (14%)
2	NAD	A	432	-	46,48,48	2.55	11 (23%)	64,73,73	1.51	10 (15%)
3	ADN	C	433	-	21,21,21	1.33	2 (9%)	31,31,31	1.37	2 (6%)
2	NAD	B	432	-	46,48,48	2.60	9 (19%)	64,73,73	1.48	9 (14%)
2	NAD	C	432	-	46,48,48	2.65	10 (21%)	64,73,73	1.52	10 (15%)
3	ADN	A	433	-	21,21,21	1.16	1 (4%)	31,31,31	1.39	3 (9%)
3	ADN	D	433	-	21,21,21	1.14	1 (4%)	31,31,31	1.34	3 (9%)

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	ADN	B	433	-	-	0/6/22/22	0/3/3/3
2	NAD	D	432	-	-	5/30/62/62	0/5/5/5
2	NAD	A	432	-	-	5/30/62/62	0/5/5/5
3	ADN	C	433	-	-	0/6/22/22	0/3/3/3
2	NAD	B	432	-	-	5/30/62/62	0/5/5/5
2	NAD	C	432	-	-	5/30/62/62	0/5/5/5
3	ADN	A	433	-	-	0/6/22/22	0/3/3/3
3	ADN	D	433	-	-	0/6/22/22	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	432	NAD	C5N-C4N	9.57	1.55	1.38
2	D	432	NAD	C5N-C4N	9.35	1.54	1.38
2	A	432	NAD	C5N-C4N	8.89	1.54	1.38
2	B	432	NAD	C5N-C4N	8.60	1.53	1.38
2	D	432	NAD	C2N-N1N	7.70	1.43	1.35
2	D	432	NAD	C4N-C3N	7.54	1.50	1.39
2	B	432	NAD	C2N-N1N	7.44	1.43	1.35
2	C	432	NAD	C2N-N1N	7.31	1.43	1.35
2	A	432	NAD	C2N-N1N	7.21	1.42	1.35
2	C	432	NAD	C4N-C3N	7.20	1.50	1.39
2	B	432	NAD	C4N-C3N	7.06	1.50	1.39
2	A	432	NAD	C4N-C3N	6.70	1.49	1.39
2	B	432	NAD	C2N-C3N	6.14	1.48	1.39
2	D	432	NAD	C2N-C3N	6.12	1.48	1.39
2	A	432	NAD	C2N-C3N	5.89	1.48	1.39
2	D	432	NAD	C6N-N1N	5.61	1.48	1.35
2	C	432	NAD	C2N-C3N	5.41	1.47	1.39
2	B	432	NAD	C6N-N1N	5.14	1.47	1.35
2	C	432	NAD	C6N-N1N	4.99	1.46	1.35
2	A	432	NAD	C6N-N1N	4.66	1.46	1.35
2	C	432	NAD	PA-O3	-4.10	1.55	1.59
2	B	432	NAD	O4B-C1B	-3.78	1.33	1.42
2	C	432	NAD	C2A-N1A	3.53	1.40	1.33
2	B	432	NAD	C2A-N1A	3.39	1.40	1.33
2	D	432	NAD	C2A-N1A	3.17	1.39	1.33
2	A	432	NAD	C2A-N1A	3.12	1.39	1.33
2	C	432	NAD	PN-O3	-2.94	1.56	1.59
2	D	432	NAD	PA-O3	-2.87	1.56	1.59
2	D	432	NAD	C7N-N7N	2.80	1.38	1.33
2	A	432	NAD	C6A-N1A	2.72	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	433	ADN	C4-N3	2.71	1.39	1.34
2	C	432	NAD	C7N-N7N	2.68	1.37	1.33
2	A	432	NAD	C7N-N7N	2.68	1.37	1.33
3	B	433	ADN	C8-N9	2.51	1.41	1.37
3	C	433	ADN	C2-N3	2.49	1.38	1.33
2	A	432	NAD	O4B-C1B	-2.43	1.36	1.42
3	B	433	ADN	C2-N3	2.25	1.37	1.33
3	B	433	ADN	C2-N1	2.24	1.37	1.33
2	A	432	NAD	PA-O3	-2.20	1.57	1.59
2	B	432	NAD	C7N-N7N	2.17	1.36	1.33
2	C	432	NAD	O4B-C1B	-2.17	1.37	1.42
3	D	433	ADN	C2-N3	2.14	1.37	1.33
2	D	432	NAD	O4B-C1B	-2.12	1.37	1.42
3	A	433	ADN	C8-N9	2.12	1.41	1.37
2	B	432	NAD	PN-O3	2.09	1.61	1.59
2	A	432	NAD	O4D-C1D	2.07	1.43	1.40
3	B	433	ADN	C5-C4	2.04	1.42	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	432	NAD	C3N-C7N-N7N	4.92	123.80	117.74
2	B	432	NAD	C3N-C7N-N7N	4.80	123.65	117.74
2	C	432	NAD	O7N-C7N-C3N	-4.79	113.74	119.60
2	A	432	NAD	C3N-C7N-N7N	4.63	123.45	117.74
2	D	432	NAD	C3N-C7N-N7N	4.57	123.37	117.74
2	A	432	NAD	O7N-C7N-C3N	-4.55	114.04	119.60
2	A	432	NAD	C6N-N1N-C2N	-4.54	118.02	121.88
2	B	432	NAD	O7N-C7N-C3N	-4.47	114.13	119.60
2	D	432	NAD	C6N-N1N-C2N	-4.45	118.09	121.88
2	D	432	NAD	O7N-C7N-C3N	-4.45	114.16	119.60
2	B	432	NAD	C6N-N1N-C2N	-4.43	118.11	121.88
2	C	432	NAD	C6N-N1N-C2N	-4.32	118.20	121.88
3	C	433	ADN	C4'-O4'-C1'	-4.28	100.02	109.47
3	D	433	ADN	C4'-O4'-C1'	-4.13	100.34	109.47
3	A	433	ADN	C4'-O4'-C1'	-4.12	100.37	109.47
2	C	432	NAD	C5N-C4N-C3N	-3.92	116.51	120.36
3	B	433	ADN	C4'-O4'-C1'	-3.78	101.12	109.47
2	A	432	NAD	C5N-C4N-C3N	-3.66	116.77	120.36
2	D	432	NAD	C5N-C4N-C3N	-3.48	116.94	120.36
2	B	432	NAD	O4B-C1B-C2B	-3.44	99.25	106.62
3	B	433	ADN	O4'-C4'-C3'	-3.14	98.92	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	433	ADN	O4'-C4'-C3'	-3.14	98.93	105.15
3	A	433	ADN	O4'-C4'-C3'	-3.13	98.94	105.15
2	B	432	NAD	C5N-C4N-C3N	-3.07	117.35	120.36
2	D	432	NAD	O4B-C1B-C2B	-3.03	100.12	106.62
2	C	432	NAD	O4B-C1B-C2B	-3.00	100.20	106.62
2	C	432	NAD	C6N-N1N-C1D	2.98	125.58	119.73
3	D	433	ADN	O4'-C4'-C3'	-2.96	99.27	105.15
2	D	432	NAD	C6N-N1N-C1D	2.80	125.21	119.73
2	A	432	NAD	O4B-C1B-C2B	-2.65	100.95	106.62
2	B	432	NAD	C5N-C6N-N1N	2.58	123.90	120.38
2	A	432	NAD	C5N-C6N-N1N	2.52	123.82	120.38
2	A	432	NAD	O5B-C5B-C4B	-2.51	100.44	108.99
2	A	432	NAD	C6N-N1N-C1D	2.48	124.59	119.73
2	D	432	NAD	C5N-C6N-N1N	2.34	123.57	120.38
2	B	432	NAD	C6N-N1N-C1D	2.28	124.21	119.73
2	B	432	NAD	O2N-PN-O5D	2.22	117.62	107.57
2	C	432	NAD	O3-PA-O1A	-2.21	104.05	110.70
2	C	432	NAD	O2A-PA-O3	2.16	113.11	107.27
2	A	432	NAD	O2A-PA-O3	2.15	113.09	107.27
2	B	432	NAD	O3-PA-O1A	-2.13	104.30	110.70
3	A	433	ADN	O4'-C1'-N9	2.12	112.17	108.09
2	A	432	NAD	O3-PA-O1A	-2.12	104.33	110.70
2	C	432	NAD	C5N-C6N-N1N	2.11	123.26	120.38
2	D	432	NAD	O3-PA-O1A	-2.11	104.36	110.70
3	D	433	ADN	O2'-C2'-C1'	2.08	117.26	110.10
2	D	432	NAD	O5B-C5B-C4B	-2.06	101.98	108.99
3	B	433	ADN	O4'-C1'-N9	2.05	112.03	108.09
2	C	432	NAD	O2N-PN-O5D	2.01	116.69	107.57

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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	C	432	NAD	O4D-C1D-N1N-C2N

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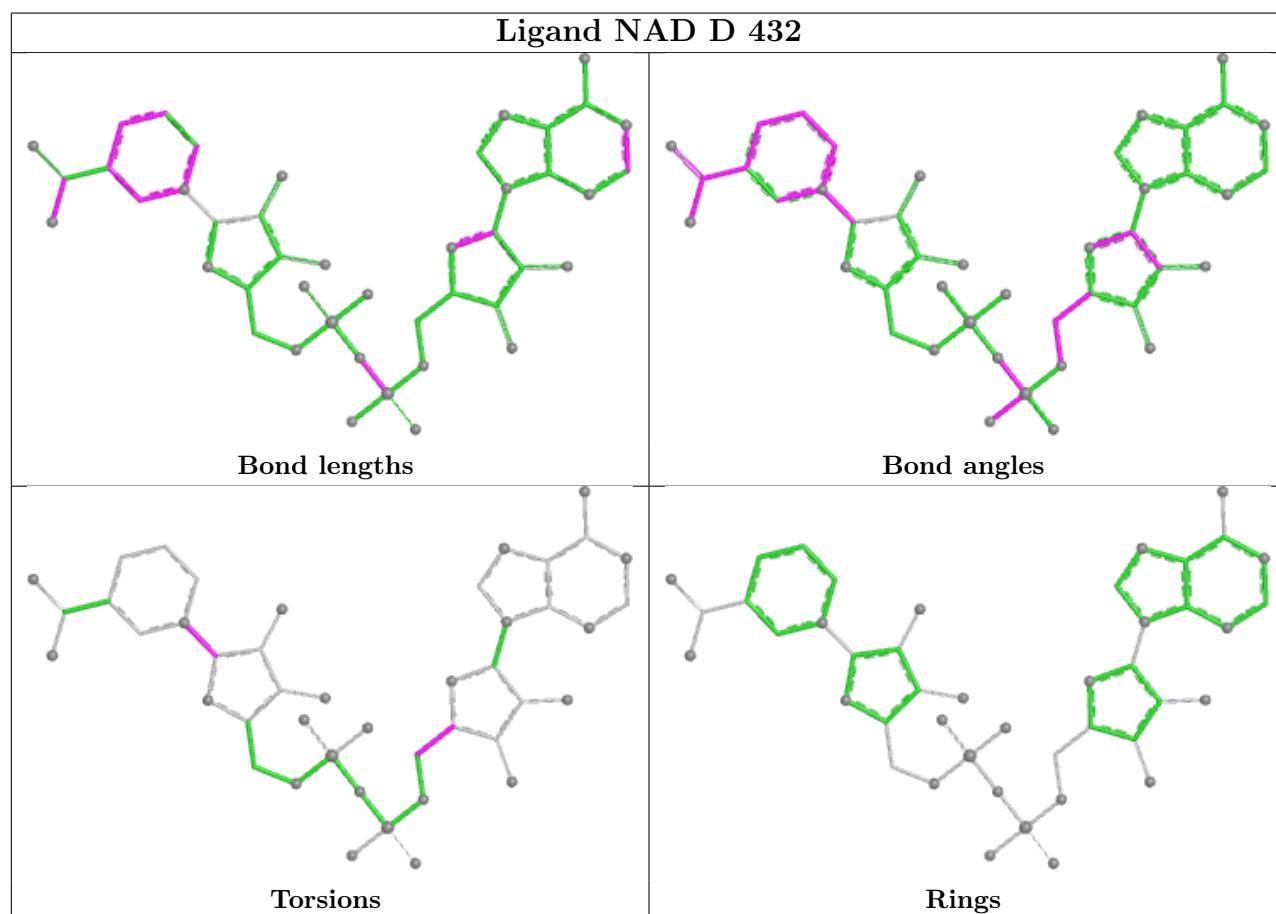
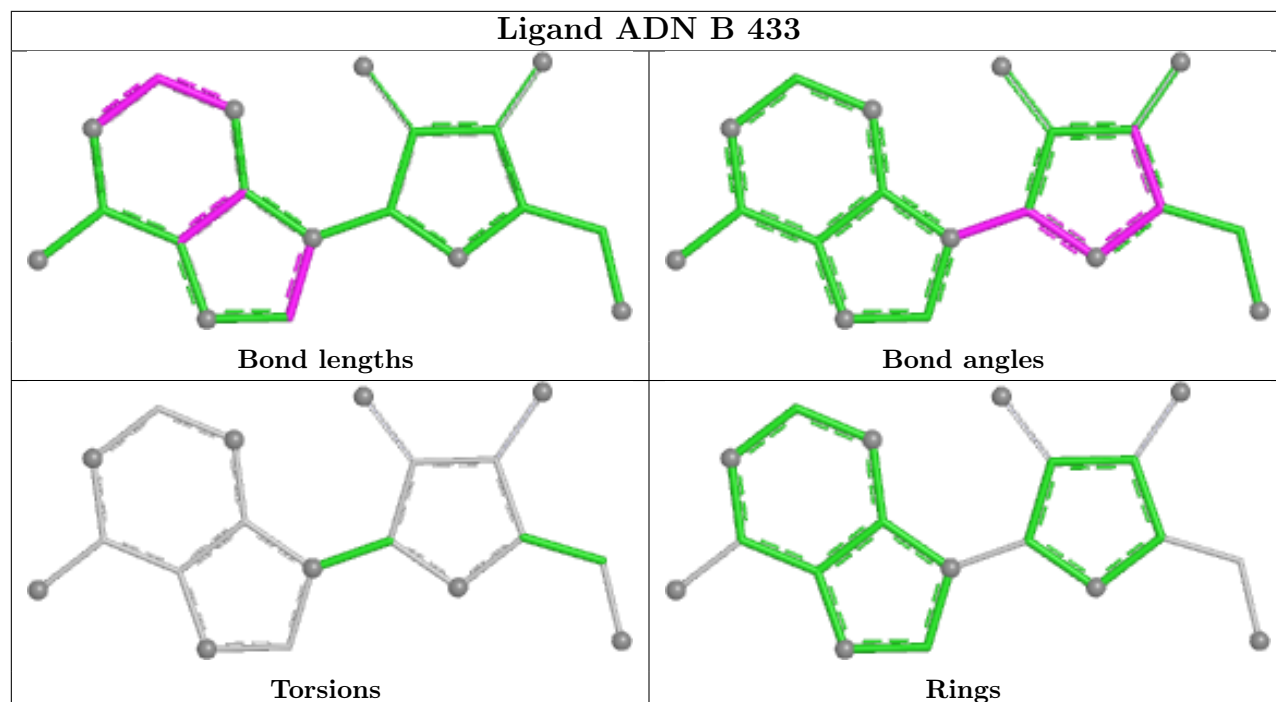
Mol	Chain	Res	Type	Atoms
2	C	432	NAD	O4D-C1D-N1N-C6N
2	C	432	NAD	C2D-C1D-N1N-C2N
2	C	432	NAD	C2D-C1D-N1N-C6N
2	D	432	NAD	O4D-C1D-N1N-C2N
2	D	432	NAD	O4D-C1D-N1N-C6N
2	D	432	NAD	C2D-C1D-N1N-C2N
2	D	432	NAD	C2D-C1D-N1N-C6N
2	C	432	NAD	O4B-C4B-C5B-O5B
2	B	432	NAD	O4B-C4B-C5B-O5B
2	D	432	NAD	O4B-C4B-C5B-O5B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

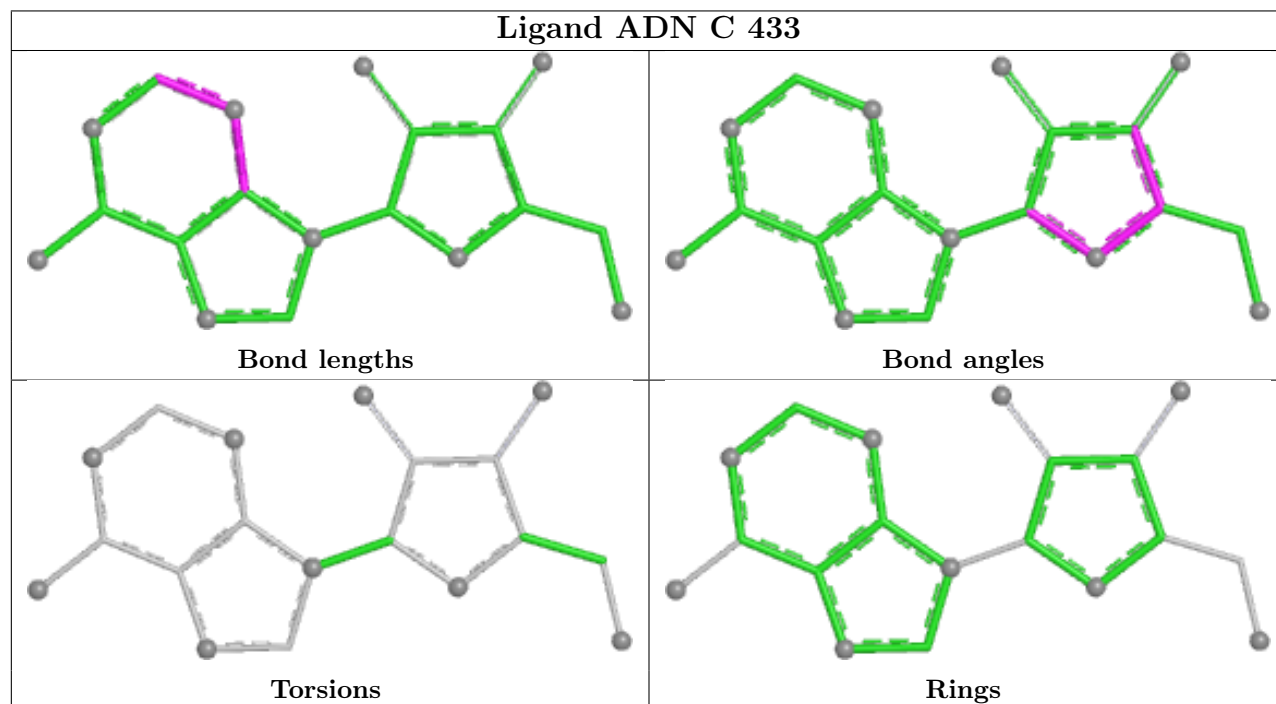
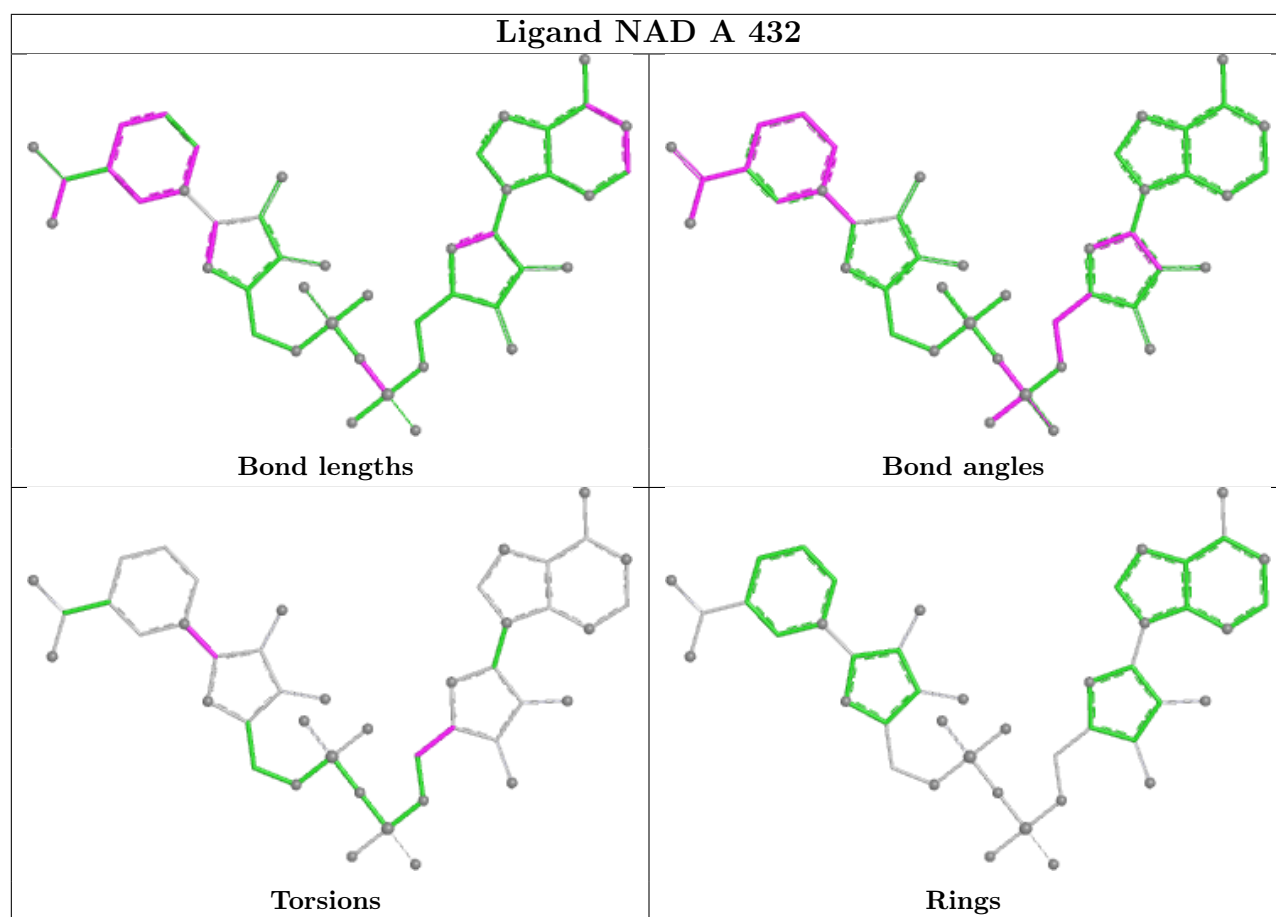
There are no ring outliers.

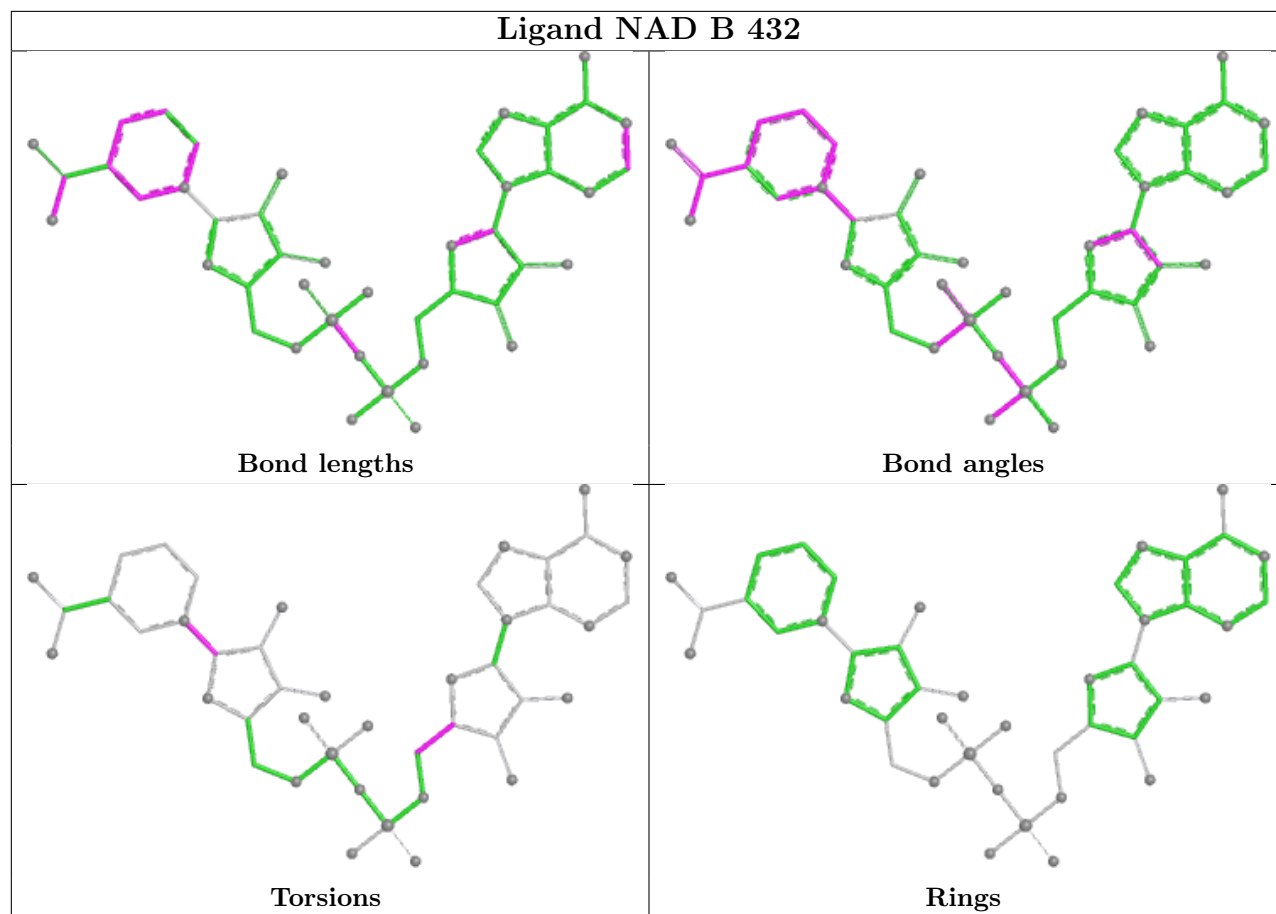
6 monomers are involved in 20 short contacts:

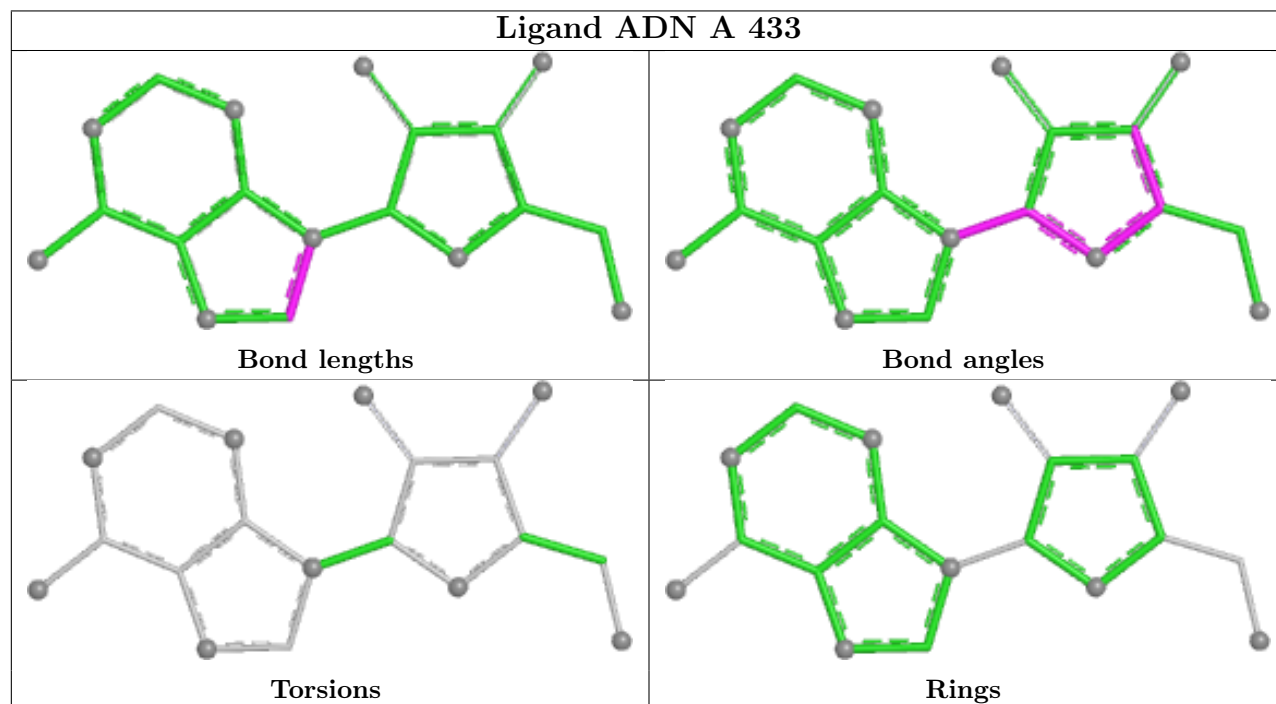
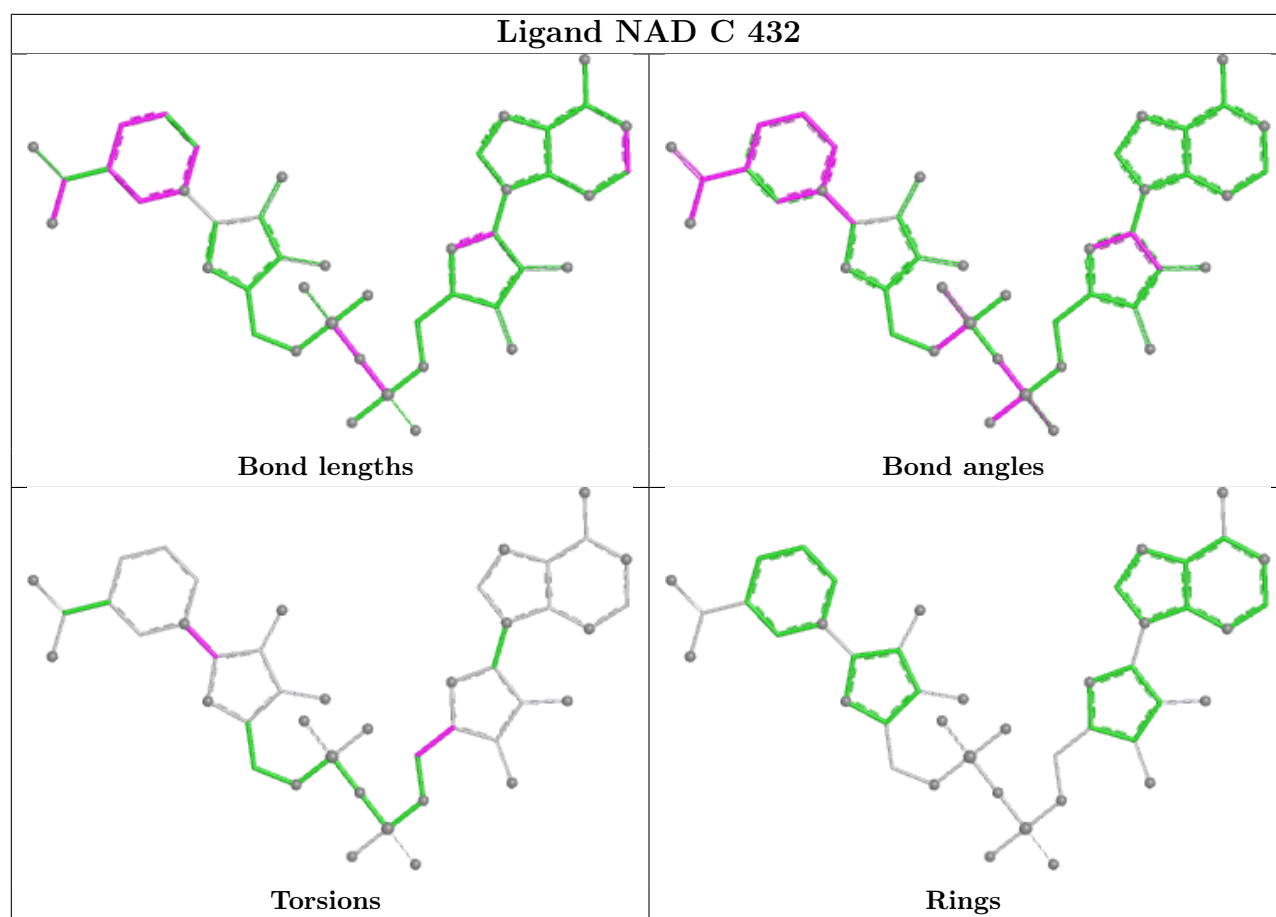
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	432	NAD	5	0
2	A	432	NAD	4	0
2	B	432	NAD	4	0
2	C	432	NAD	5	0
3	A	433	ADN	1	0
3	D	433	ADN	1	0

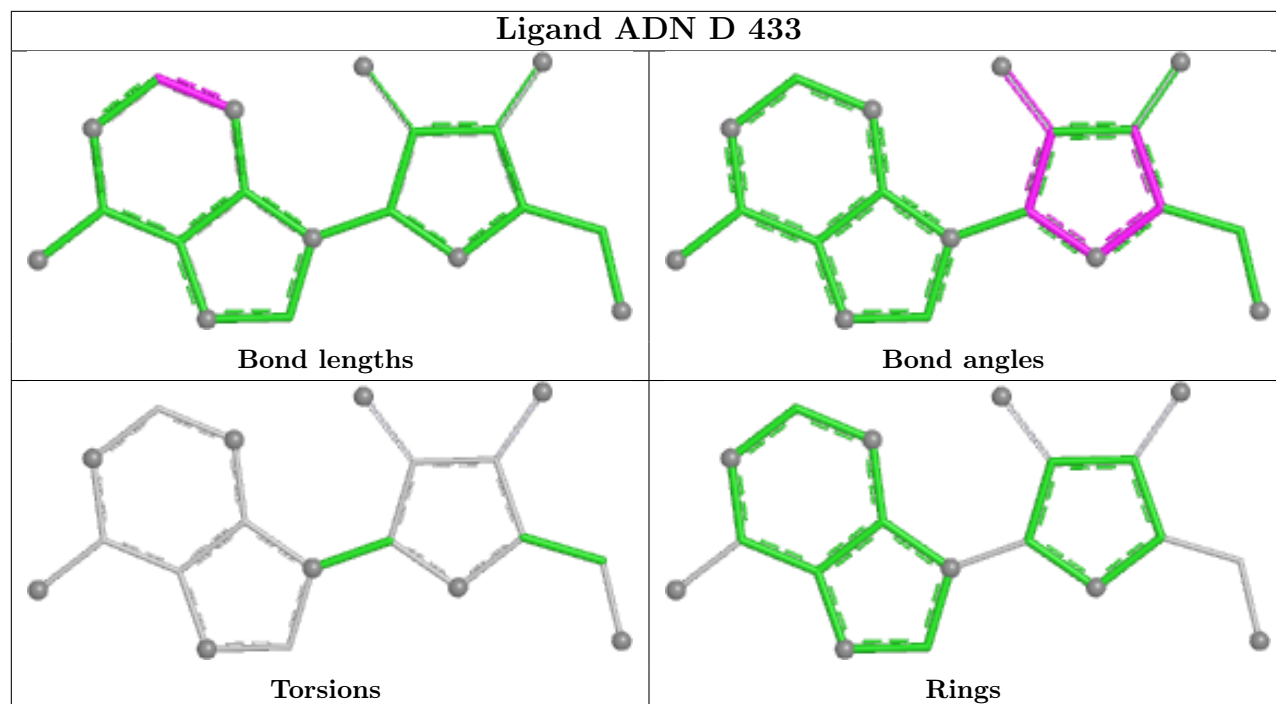
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	430/431 (99%)	-1.80	0 100 100	2, 26, 49, 73	0
1	B	430/431 (99%)	-1.81	0 100 100	4, 26, 51, 73	0
1	C	430/431 (99%)	-1.79	0 100 100	3, 28, 50, 73	0
1	D	430/431 (99%)	-1.78	0 100 100	3, 28, 51, 75	0
All	All	1720/1724 (99%)	-1.79	0 100 100	2, 27, 51, 75	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

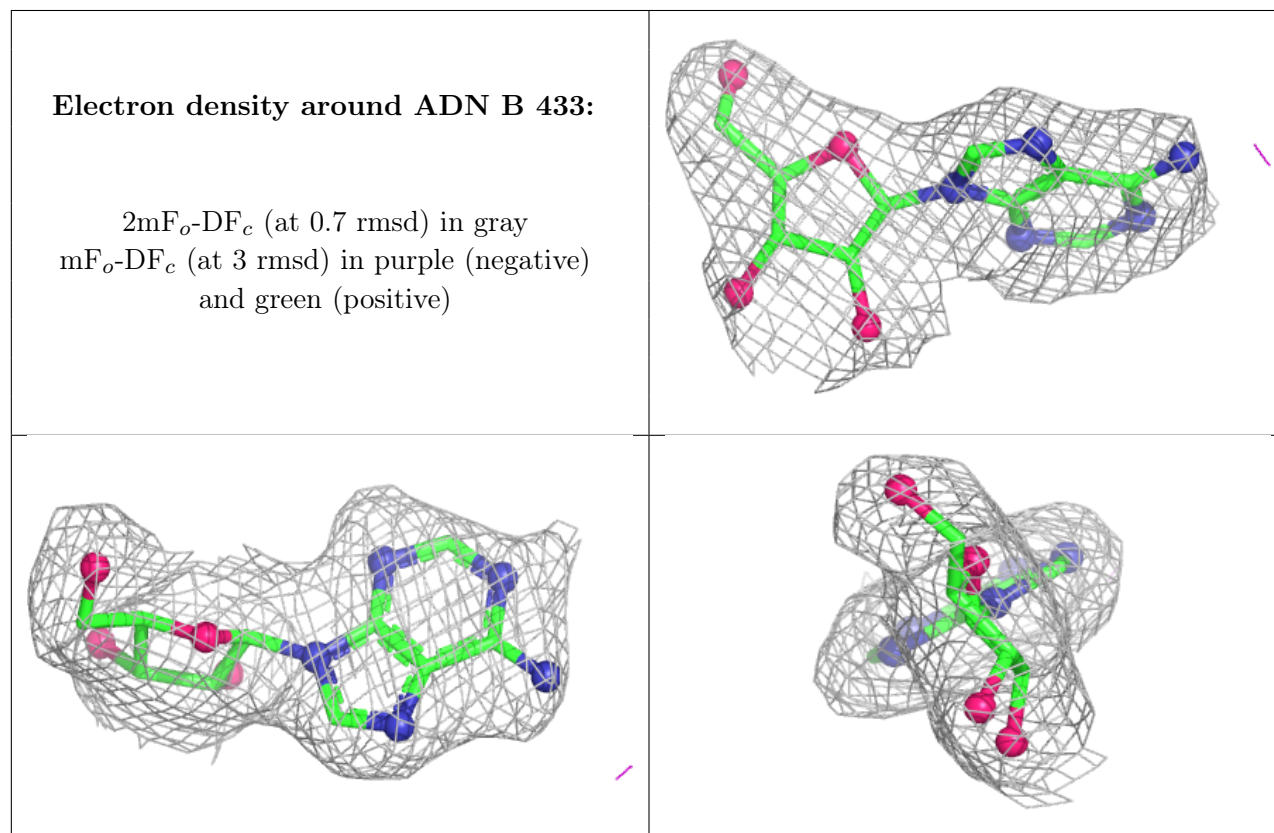
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADN	B	433	19/19	0.99	0.03	13,18,22,25	0
3	ADN	C	433	19/19	0.99	0.03	10,16,27,30	0
2	NAD	C	432	44/44	1.00	0.02	5,14,22,25	0
2	NAD	D	432	44/44	1.00	0.02	2,17,21,23	0

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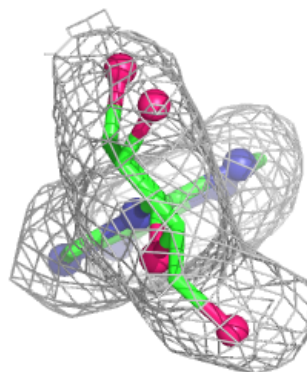
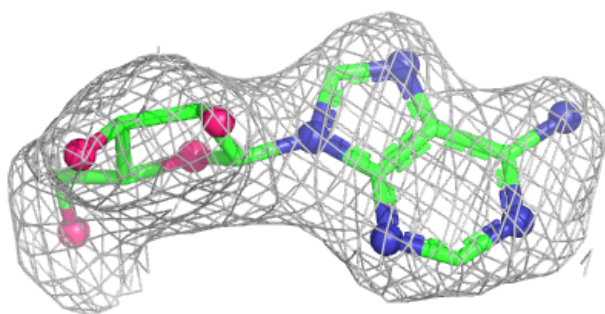
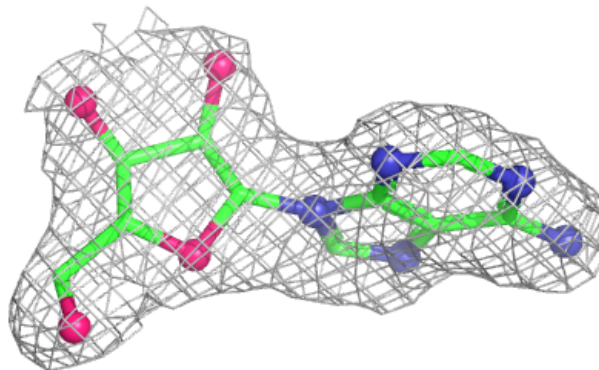
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADN	A	433	19/19	1.00	0.02	12,17,24,33	0
2	NAD	A	432	44/44	1.00	0.02	2,16,21,23	0
2	NAD	B	432	44/44	1.00	0.03	2,8,16,24	0
3	ADN	D	433	19/19	1.00	0.03	10,18,23,26	0

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.

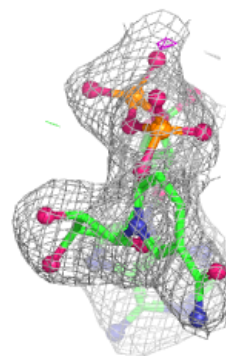
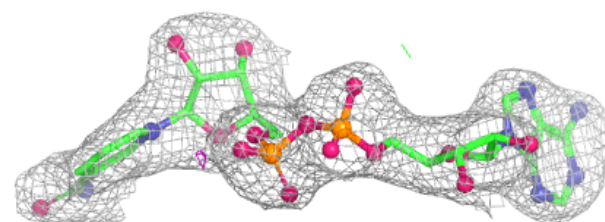
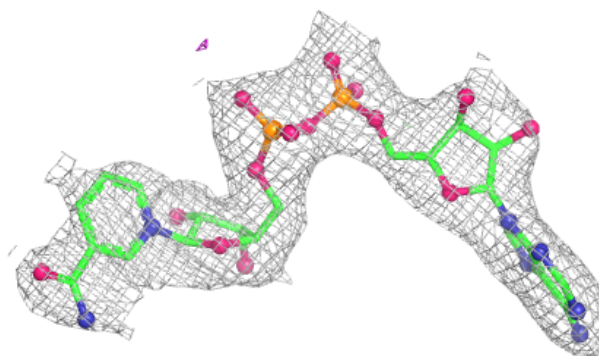


Electron density around ADN C 433:

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

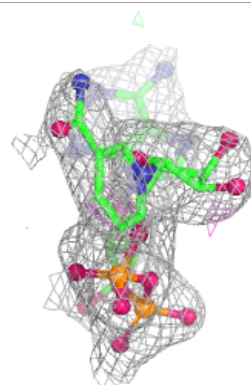
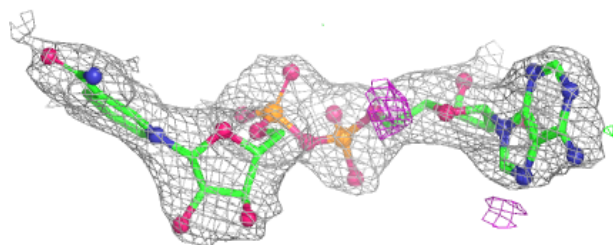
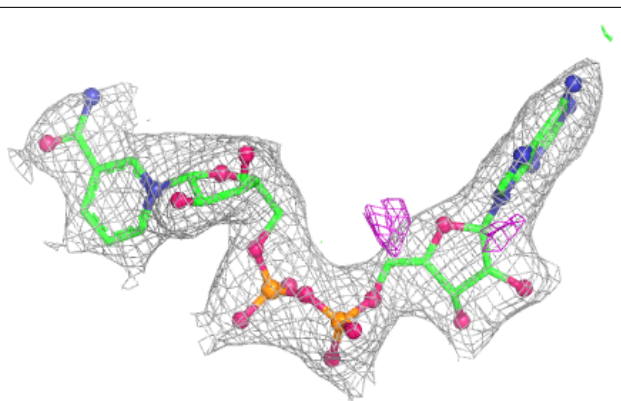
**Electron density around NAD C 432:**

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

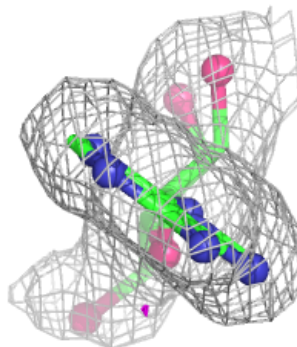
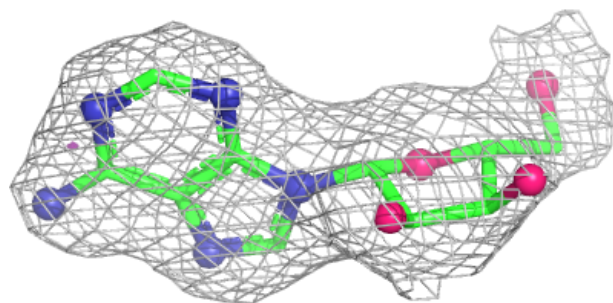
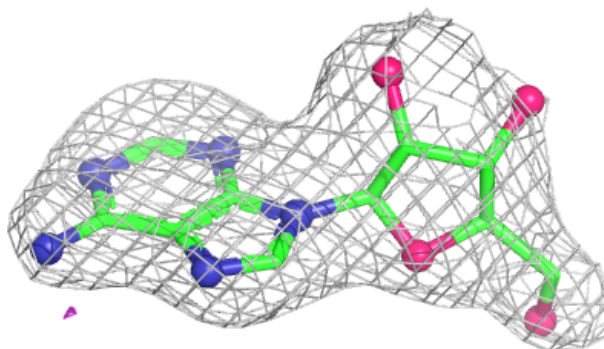


Electron density around NAD D 432:

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and green (positive)

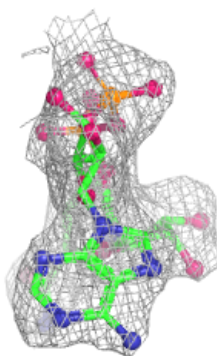
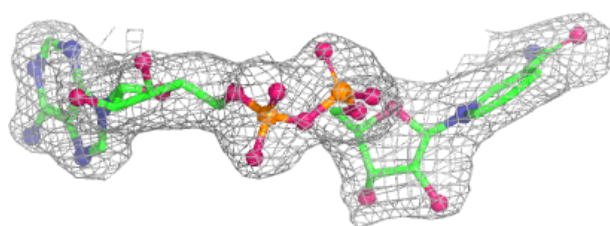
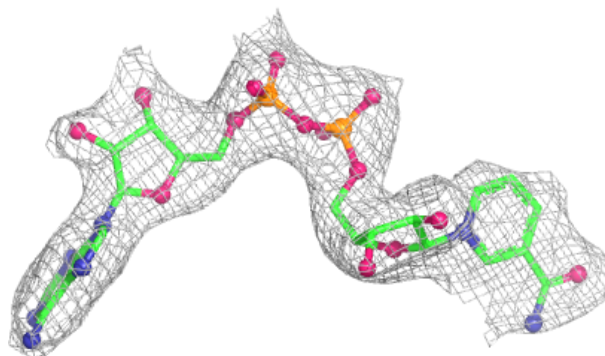
**Electron density around ADN A 433:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

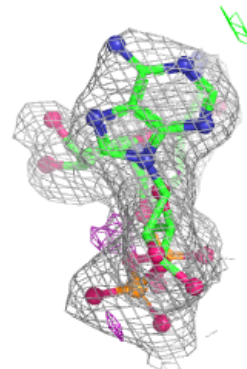
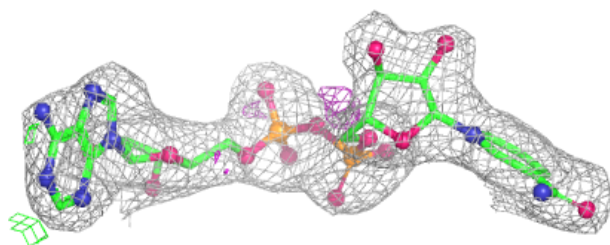
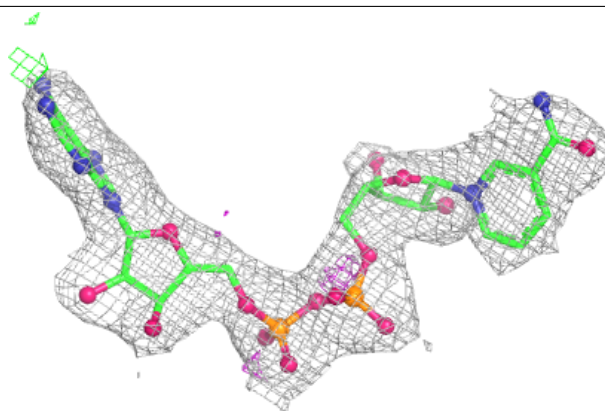


Electron density around NAD A 432:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

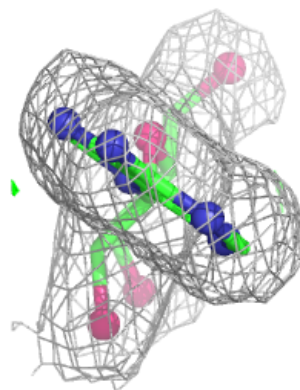
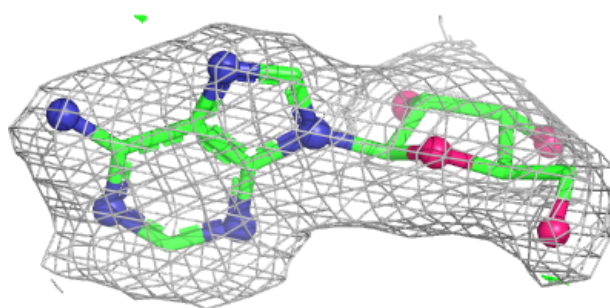
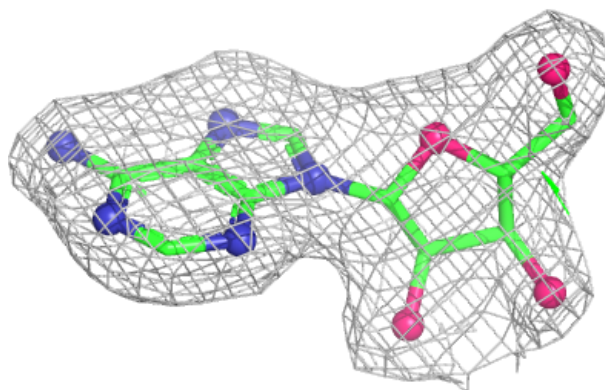
**Electron density around NAD B 432:**

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



Electron density around ADN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.