Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 05:40 AM EST

PDB ID	:	1XLT
Title	:	Crystal structure of Transhydrogenase [(domain I)2:domain III] heterotrimer complex
Authors	:	Sundaresan, V.; Chartron, J.; Yamaguchi, M.; Stout, C.D.
Deposited on	:	2004-09-30
Resolution	:	3.10 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:

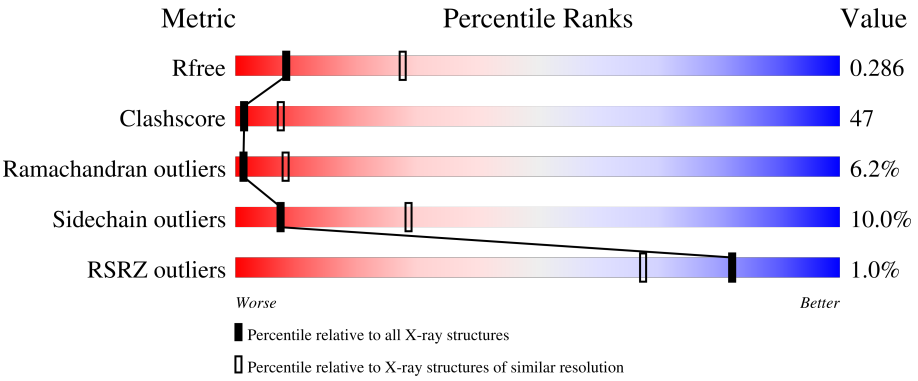
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	384	42% 44% 8% • 5%
1	B	384	39% 43% 11% • 7%
1	D	384	29% 54% 13% • •
1	E	384	33% 51% 8% • 7%
1	G	384	38% 49% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	H	384	3% 26% 54% 12% 7%
2	C	174	43% 51% 6%
2	F	174	44% 50% 5%
2	I	174	34% 55% 9%
3	J	2	100%
3	K	2	50% 50%
3	L	2	100%
3	M	2	100%
3	N	2	100%
3	O	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	N	1	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20480 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 NAD(P) transhydrogenase subunit alpha part 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2670	1688	462	504	16			
1	B	359	Total	C	N	O	S	0	0	0
			2643	1673	458	496	16			
1	D	378	Total	C	N	O	S	0	0	0
			2779	1753	479	529	18			
1	E	359	Total	C	N	O	S	0	0	0
			2644	1673	458	497	16			
1	G	364	Total	C	N	O	S	0	0	0
			2675	1691	463	505	16			
1	H	357	Total	C	N	O	S	0	0	0
			2632	1665	456	495	16			

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1318	833	221	252	12			
2	F	173	Total	C	N	O	S	0	0	0
			1307	827	217	251	12			
2	I	173	Total	C	N	O	S	0	0	0
			1307	827	217	251	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	291	ARG	-	cloning artifact	UNP Q59765
C	292	HIS	-	cloning artifact	UNP Q59765
C	293	MET	-	cloning artifact	UNP Q59765
F	291	ARG	-	cloning artifact	UNP Q59765
F	292	HIS	-	cloning artifact	UNP Q59765
F	293	MET	-	cloning artifact	UNP Q59765

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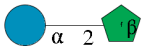
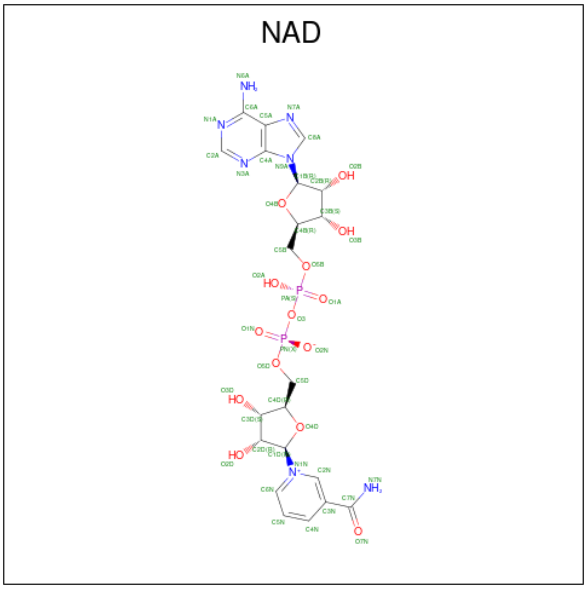
Chain	Residue	Modelled	Actual	Comment	Reference
I	291	ARG	-	cloning artifact	UNP Q59765
I	292	HIS	-	cloning artifact	UNP Q59765
I	293	MET	-	cloning artifact	UNP Q59765

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	2	Total C O 23 12 11	0	0	0
3	K	2	Total C O 23 12 11	0	0	0
3	L	2	Total C O 23 12 11	0	0	0
3	M	2	Total C O 23 12 11	0	0	0
3	N	2	Total C O 23 12 11	0	0	0
3	O	2	Total C O 23 12 11	0	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

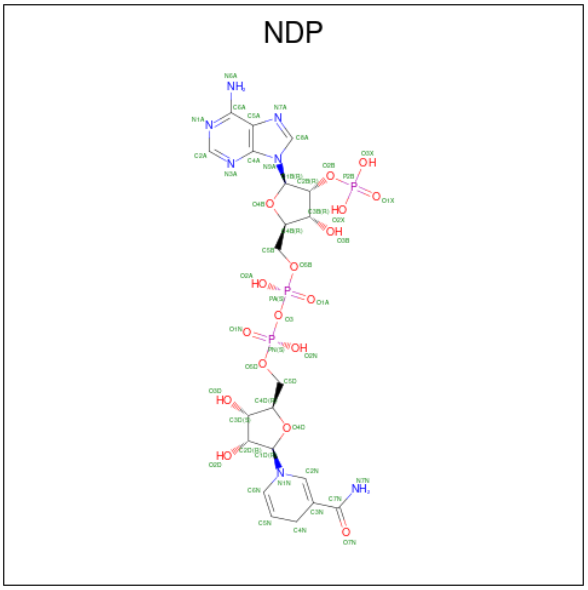


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		
5	G	1	Total	Na	0	0
			1	1		

- Molecule 6 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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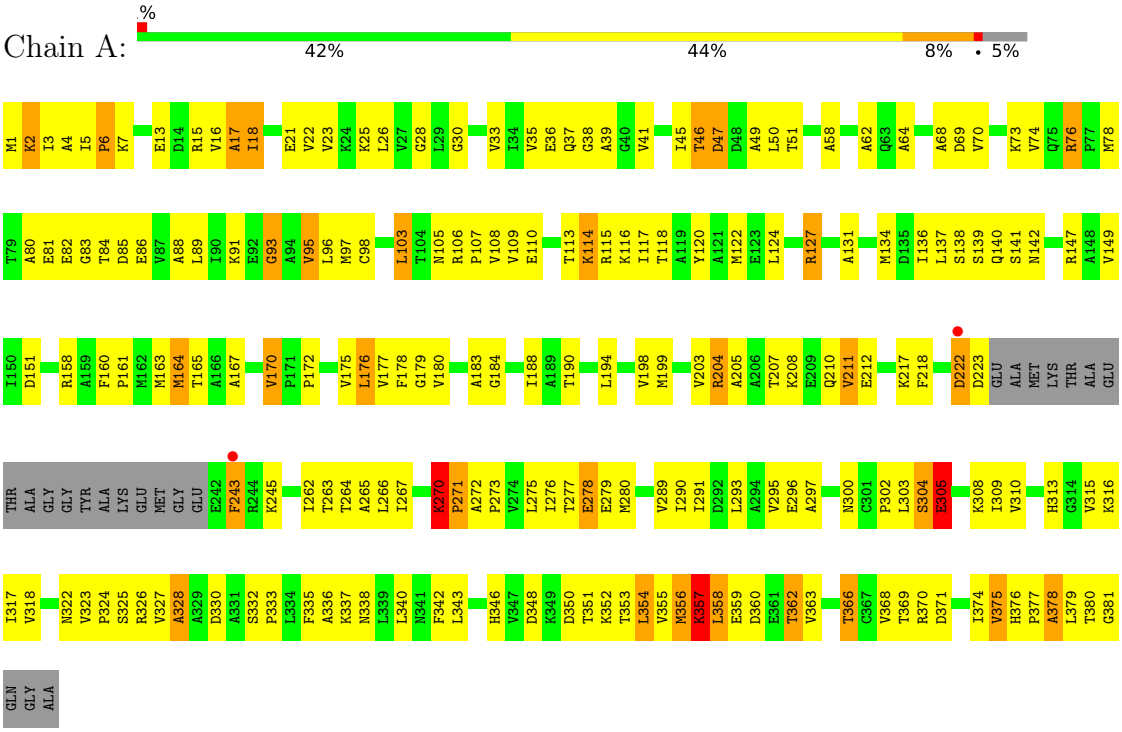
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
6	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

3 Residue-property plots (i)

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

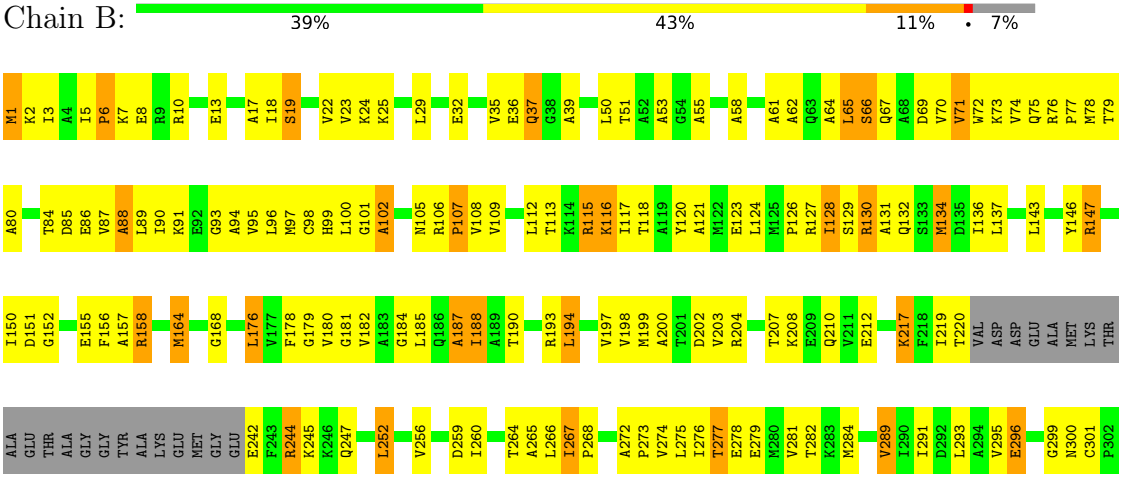
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

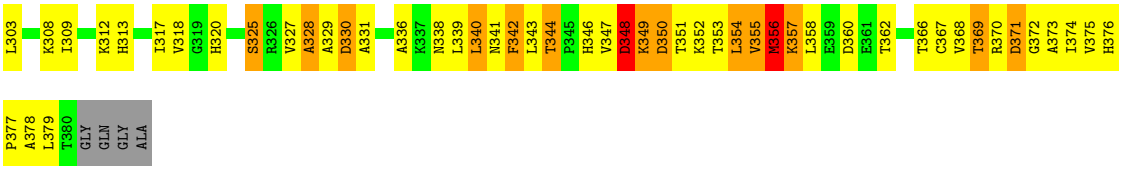
Chain A:



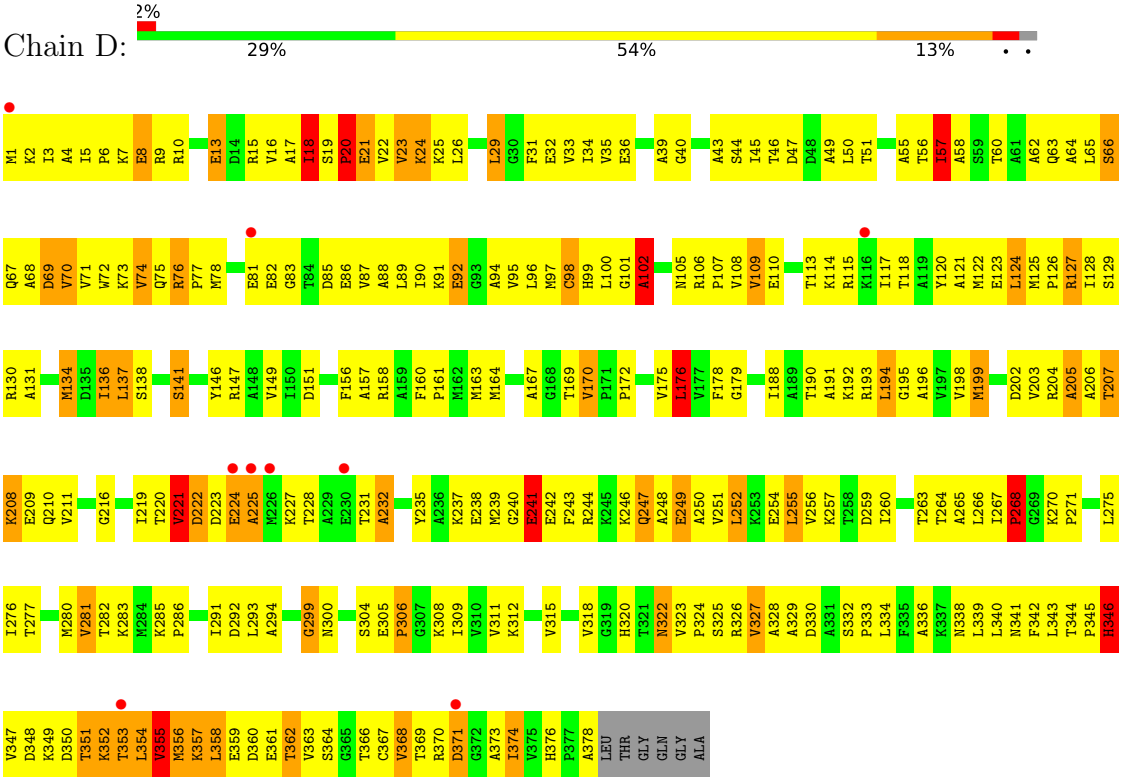
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain B:

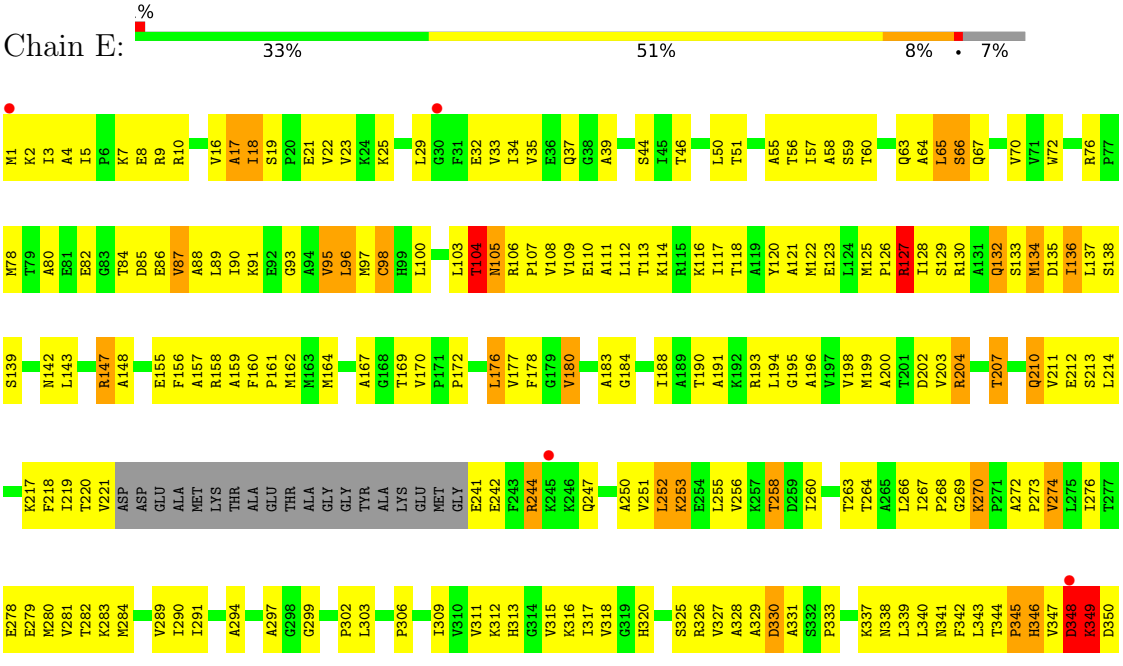




• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



T351 K352 T353 L354 V355 M356 K357 L358 E359 D360 E361 T362 V363 S364 G365 T366 C367 V368 T369 R370 D371 G372 A373 I374 V375 A378 LEU THR GLY GLN GLY ALA

• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain G: 38% 49% 8% • 5%

M1 K2 I3 A4 I5 P6 K7 E8 R9 R10 P11 G12 E13 D14 R15 V16 A17 I18 S19 P20 E21 V22 V23 L26 V27 G28 L29 G30 F31 E32 V33 I34 V35 E36 Q37 G38 A39 G40 V41 I45 T46 D47 L50 T51 A55 T56 I57 A58 S59 T60 A61 A62 Q63 A64 L65 S66
Q67 A68 D69 V70 V71 W72 K73 V74 Q75 R76 P77 M78 E82 D85 E86 V87 A88 L89 I90 K91 E92 G93 A94 V95 L96 M97 C98 H99 L100 G101 A102 L103 T104 N105 R106 P107 E110 A111 L112 T113 K114 R115 K116 I117 T118 A119 Y120 A121 M122 E123 L124 I128 S129 R130 A131 Q132
S133 I136 L137 S138 S139 A153 Y154 E155 F156 A157 R158 A159 F160 P161 M162 M163 M164 T165 A166 V170 P171 P172 A173 R174 V175 L176 V177 F178 G179 V180 G181 V182 A183 G184 L185 I188 K192 R193 L194 V198 M199 A200 V203 R204 T207 K208 V211 E212 S213 L214
K217 F218 I219 T220 V221 D222 ASP GLU ALA MET LYS THR ALA GLU THR ALA GLY GLY TYR ALA LYS GLU MET G240 F243 R244 K245 K246 Q247 A248 E249 L252 L255 V256 K257 T258 D259 I260 T263 T264 A265 L266 K270 P273 V274 L275 I276 T277 E278 E279 M280 V281 T282 K283
M284 K285 V289 I290 I291 D292 L293 A294 V295 G299 N300 C301 P302 L303 P306 G307 K308 I309 V310 V311 K312 H313 G314 V315 K316 I317 V318 N322 R326 A329 D330 A331 S332 P333 L334 N338 L339 L340 N341 F342 L343 T344 P345 H346 V347 D348 K349 D350 T351 K352 T353 L354 V355
M356 K357 L358 E359 D360 E361 T362 V363 T366 C367 V368 T369 R370 D371 G372 A373 I374 V375 H376 P377 A378 L379 T380 G381 GLN GLY ALA

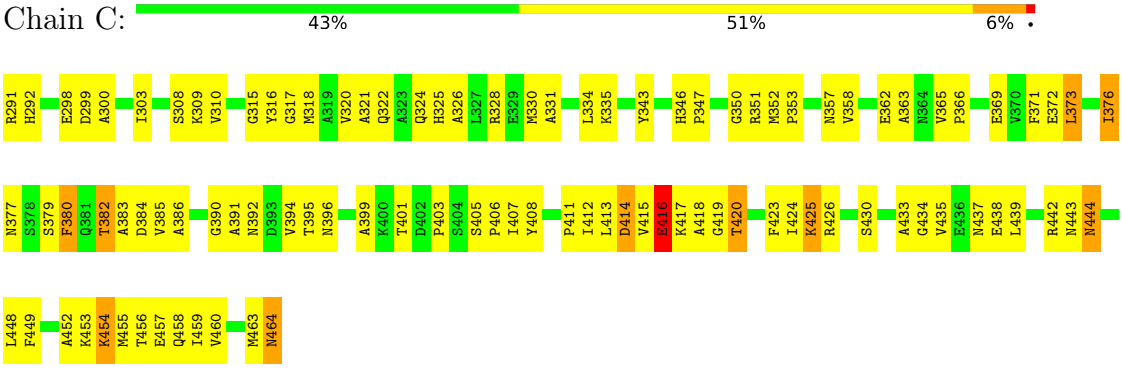
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain H: 3% 26% 54% 12% • 7%

M1 K2 I3 A4 I5 P6 K7 E8 R9 R10 P11 G12 E13 D14 R15 V16 A17 I18 S19 V22 V23 K24 K25 L26 V27 G28 L29 G30 F31 E32 V33 I34 V35 E36 Q37 G38 A39 G40 V41 G42 A43 T46 D47 D48 A49 L50 T51 A52 A53 G54 A55 T56 I57 A58 S59 T60 A61 A62
Q63 A64 L65 S66 Q67 A68 D69 V70 V71 W72 K73 V74 Q75 R76 P77 M78 E81 E82 D85 E86 V87 A88 L89 I90 K91 E92 G93 A94 V95 L96 M97 C98 H99 L100 G101 A102 L103 T104 N105 R106 V109 E110 A111 L112 T113 K114 R115 K116 I117 T118 A119 Y120 A121 M122 E123 L124 M125
P126 R127 I128 S129 R130 A131 Q132 S133 M134 D135 I136 L137 N142 L143 Y146 R147 A148 D151 F156 A157 R158 A159 F160 P161 M162 M163 M164 T169 V170 P171 P172 L176 V177 F178 G179 V180 G181 V182 A183 G184 L185 Q186 A187 I188 K192 R193 L194 G195 A196 M199 D202
V203 R204 A205 A206 T207 K208 E209 Q210 V211 E212 S213 L214 G215 F218 I219 T220 VAL ASP ASP GLU ALA MET LYS THR ALA GLU THR ALA GLY GLY TYR ALA LYS GLU MET GLY E241 E242 F243 R244 K245 K246 Q247 A248 E249 A250 V251 L252 A261 I262 T263 T264 A265 L266 I267 P268 G269 K270
P271 A272 P273 V274 L275 I276 T277 E278 E279 M280 V281 T282 K283 M284 K285 P286 I290 I291 D292 L293 A294 V295 E296 A297 G298 G299 N300 C301 P302 L303 S304 I309 V310 V311 K312 H313 G314 V315 K316 I317 V318 G319 H320 T321 N322 V323 P324 S325 R326 V327 D330 A331 S332 P333 L334 F335 A336
K337 N338 L339 L340 N341 F342 L343 T344 P345 H346 V347 D348 K349 K352 T353 L354 V355 M356 K357 L358 E359 D360 E361 T362 V363 S364 G365 T366 C367 V368 T369 R370 D371 G372 A373 I374 V375 H376 P377 ALA LEU THR GLY GLN GLY ALA

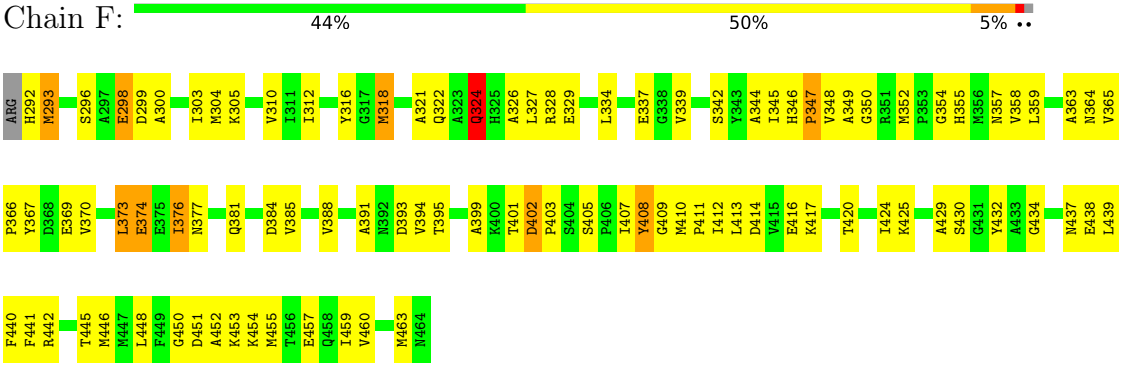
• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain C:



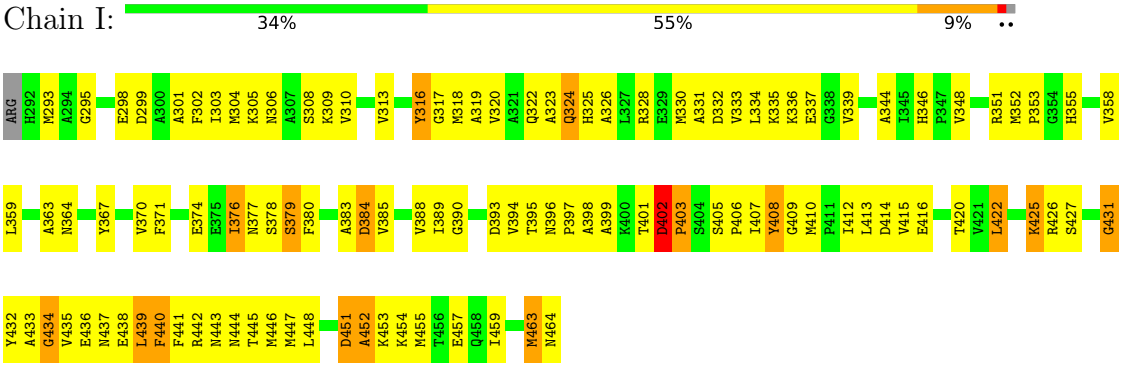
• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain F:



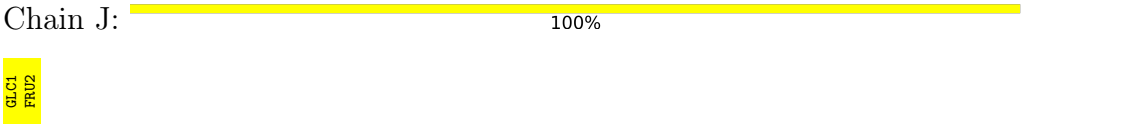
• Molecule 2: NAD(P) transhydrogenase subunit beta

Chain I:



• Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain J:

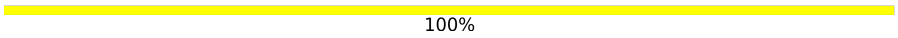


• Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain K:

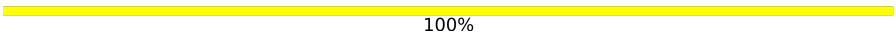
• Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain L:



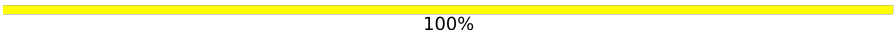
• Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain M:



• Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain N:



• Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.37Å 171.08Å 203.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 3.10 43.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.68-3.10) 95.9 (43.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.310 0.220 , 0.286	Depositor DCC
R_{free} test set	2977 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	78.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20480	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: NA, FRU, NAD, NDP, GLC

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	0.52	1/2705 (0.0%)	0.82	4/3668 (0.1%)
1	B	0.48	0/2678	0.79	2/3631 (0.1%)
1	D	0.54	0/2816	1.02	10/3816 (0.3%)
1	E	0.50	1/2679 (0.0%)	0.87	7/3632 (0.2%)
1	G	0.46	0/2710	0.81	5/3674 (0.1%)
1	H	0.54	1/2667 (0.0%)	0.99	14/3615 (0.4%)
2	C	0.46	0/1342	0.66	0/1813
2	F	0.46	0/1331	0.65	0/1799
2	I	0.51	0/1331	0.85	3/1799 (0.2%)
All	All	0.50	3/20259 (0.0%)	0.86	45/27447 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	5
1	E	0	1
1	H	1	2
2	I	0	1
All	All	1	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	ARG	N-CA	-8.40	1.29	1.46
1	H	343	LEU	C-N	-6.48	1.19	1.34
1	E	349	LYS	C-O	6.47	1.35	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	125	MET	C-N-CD	9.48	148.30	128.40
1	D	371	ASP	CB-CG-OD2	8.76	126.18	118.30
1	A	47	ASP	CB-CG-OD1	8.75	126.18	118.30
1	D	221	VAL	O-C-N	8.62	136.49	122.70
1	G	350	ASP	CB-CG-OD2	8.56	126.01	118.30
1	H	371	ASP	CB-CG-OD2	8.45	125.91	118.30
2	I	403	PRO	CA-N-CD	-8.24	99.97	111.50
1	H	375	VAL	N-CA-C	8.14	132.97	111.00
1	E	348	ASP	C-N-CA	-8.07	101.53	121.70
1	E	348	ASP	CB-CG-OD2	-7.77	111.31	118.30
2	I	402	ASP	CB-CG-OD1	7.72	125.25	118.30
1	H	126	PRO	CA-N-CD	-7.67	100.77	111.50
1	D	67	GLN	O-C-N	-7.58	110.58	122.70
1	H	345	PRO	CA-N-CD	-7.38	101.17	111.50
1	H	342	PHE	CB-CG-CD2	6.95	125.67	120.80
1	G	357	LYS	O-C-N	-6.89	111.68	122.70
1	H	344	THR	C-N-CD	6.72	142.51	128.40
1	G	357	LYS	C-N-CA	6.51	137.99	121.70
1	B	330	ASP	CB-CG-OD1	6.45	124.10	118.30
1	D	346	HIS	CA-CB-CG	6.43	124.53	113.60
1	E	349	LYS	CA-C-N	6.37	131.22	117.20
2	I	402	ASP	CA-C-O	6.22	133.16	120.10
1	E	356	MET	CA-CB-CG	5.97	123.45	113.30
1	E	317	ILE	O-C-N	-5.96	113.17	122.70
1	H	343	LEU	C-N-CA	5.92	136.51	121.70
1	D	374	ILE	CA-C-O	5.89	132.47	120.10
1	H	133	SER	O-C-N	-5.86	113.33	122.70
1	D	220	THR	O-C-N	-5.57	113.78	122.70
1	H	365	GLY	C-N-CA	5.56	135.60	121.70
1	A	356	MET	C-N-CA	5.52	135.51	121.70
1	H	127	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	H	344	THR	N-CA-C	5.43	125.67	111.00
1	D	225	ALA	CB-CA-C	5.34	118.11	110.10
1	D	225	ALA	N-CA-CB	5.34	117.57	110.10
1	E	349	LYS	CB-CA-C	5.29	120.98	110.40
1	H	366	THR	CA-CB-CG2	5.28	119.79	112.40
1	E	297	ALA	CB-CA-C	5.23	117.94	110.10
1	A	17	ALA	CB-CA-C	5.22	117.93	110.10
1	H	126	PRO	N-CD-CG	5.21	111.02	103.20
1	A	357	LYS	C-N-CA	5.16	134.59	121.70
1	B	356	MET	O-C-N	-5.14	114.48	122.70
1	G	352	LYS	CA-C-O	5.11	130.82	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	57	ILE	C-N-CA	5.10	134.46	121.70
1	G	357	LYS	CA-C-N	5.07	128.34	117.20
1	D	69	ASP	CB-CG-OD2	5.06	122.85	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	366	THR	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ILE	Mainchain
1	B	356	MET	Mainchain
1	D	102	ALA	Mainchain
1	D	247	GLN	Mainchain
1	D	346	HIS	Sidechain
1	D	353	THR	Mainchain
1	D	57	ILE	Mainchain
1	E	356	MET	Mainchain
1	H	132	GLN	Mainchain
1	H	343	LEU	Mainchain
2	I	398	ALA	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2670	0	2804	200	0
1	B	2643	0	2784	248	0
1	D	2779	0	2904	367	0
1	E	2644	0	2781	268	0
1	G	2675	0	2808	241	0
1	H	2632	0	2766	391	0
2	C	1318	0	1305	109	0
2	F	1307	0	1292	92	0
2	I	1307	0	1292	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	23	0	21	0	0
3	K	23	0	21	1	0
3	L	23	0	21	0	0
3	M	23	0	21	0	0
3	N	23	0	21	0	0
3	O	23	0	21	1	0
4	A	44	0	26	2	0
4	B	44	0	25	9	0
4	D	44	0	24	3	0
4	G	44	0	24	6	0
4	H	44	0	26	8	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
6	C	48	0	26	4	0
6	F	48	0	26	10	0
6	I	48	0	26	3	0
All	All	20480	0	21065	1966	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 47.

All (1966) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:120:TYR:CD2	1:H:366:THR:HG22	1.64	1.31
1:H:120:TYR:HD2	1:H:366:THR:CG2	1.47	1.27
2:I:401:THR:O	2:I:403:PRO:HD3	1.32	1.25
1:B:70:VAL:HG23	1:B:95:VAL:HB	1.21	1.17
1:H:120:TYR:CD2	1:H:366:THR:CG2	2.26	1.15
1:D:62:ALA:HA	1:D:89:LEU:HD21	1.16	1.11
1:H:18:ILE:HD11	1:H:23:VAL:HG22	1.23	1.10
1:H:120:TYR:HD2	1:H:366:THR:HG22	0.94	1.09
1:B:264:THR:HG22	1:B:293:LEU:HD12	1.33	1.08
1:B:29:LEU:HD23	1:B:347:VAL:HG11	1.35	1.08
1:B:86:GLU:HA	1:B:89:LEU:HD12	1.37	1.07
1:A:270:LYS:HB2	1:A:271:PRO:HD3	1.37	1.06
1:H:47:ASP:HB3	1:H:57:ILE:HD13	1.34	1.05
1:H:72:TRP:HB3	1:H:97:MET:HB2	1.34	1.04
1:H:47:ASP:HB3	1:H:57:ILE:CD1	1.87	1.04
1:D:68:ALA:O	1:D:91:LYS:HD3	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:SER:HA	1:H:132:GLN:HG3	1.39	1.04
1:H:370:ARG:CG	1:H:375:VAL:HG21	1.88	1.04
1:D:69:ASP:O	1:D:94:ALA:HB1	1.59	1.01
1:H:370:ARG:HG2	1:H:375:VAL:CG2	1.88	1.01
1:H:47:ASP:CB	1:H:57:ILE:HD13	1.91	1.01
1:A:354:LEU:HD21	1:A:356:MET:HE2	1.39	1.00
1:H:186:GLN:HA	2:I:352:MET:HE1	1.39	1.00
1:D:361:GLU:HA	1:D:364:SER:HB3	1.43	0.99
1:B:128:ILE:CD1	1:B:130:ARG:HD3	1.92	0.99
1:H:370:ARG:HG2	1:H:375:VAL:HG21	1.00	0.99
1:H:362:THR:HG23	1:H:363:VAL:H	1.26	0.99
1:A:46:THR:HG23	1:A:49:ALA:HB2	1.44	0.98
1:D:73:LYS:O	1:D:98:CYS:HB2	1.65	0.97
1:H:121:ALA:HB1	1:H:123:GLU:OE1	1.63	0.97
1:A:270:LYS:HB2	1:A:271:PRO:CD	1.95	0.96
1:A:76:ARG:HH21	1:A:76:ARG:HG2	1.26	0.96
1:E:217:LYS:H	1:E:217:LYS:HD2	1.27	0.96
1:H:8:GLU:HG2	1:H:74:VAL:HG22	1.46	0.96
2:C:399:ALA:HB2	2:C:407:ILE:HG13	1.46	0.96
1:E:176:LEU:HB2	1:E:258:THR:HG21	1.45	0.95
1:H:74:VAL:HG23	1:H:75:GLN:H	1.29	0.95
1:E:199:MET:HG3	1:E:219:ILE:HD11	1.48	0.95
1:B:61:ALA:O	1:B:65:LEU:HD13	1.68	0.94
2:F:399:ALA:HA	2:F:408:TYR:HA	1.46	0.94
1:G:35:VAL:HG21	1:G:50:LEU:HD13	1.49	0.93
1:H:129:SER:CA	1:H:132:GLN:HG3	1.98	0.93
2:F:432:TYR:CD2	6:F:500:NDP:H1D	2.03	0.93
1:H:357:LYS:HB3	1:H:360:ASP:HB2	1.49	0.93
2:I:437:ASN:HB3	2:I:440:PHE:CE1	2.04	0.93
1:E:184:GLY:O	1:E:188:ILE:HG12	1.69	0.93
1:D:358:LEU:HD13	1:D:370:ARG:HH22	1.34	0.93
1:G:85:ASP:OD2	1:G:88:ALA:HB2	1.68	0.93
1:D:342:PHE:CZ	1:D:362:THR:O	2.22	0.93
1:H:354:LEU:HD23	1:H:354:LEU:H	1.32	0.93
1:B:128:ILE:HD12	1:B:130:ARG:HD3	1.47	0.92
1:E:188:ILE:HG23	1:E:198:VAL:HG11	1.52	0.92
1:G:120:TYR:HB3	1:G:366:THR:HG22	1.52	0.92
1:B:349:LYS:HG3	1:B:350:ASP:H	1.33	0.92
1:G:78:MET:HB2	1:G:86:GLU:HG3	1.52	0.92
1:G:329:ALA:HB3	1:H:158:ARG:HG2	1.52	0.92
1:D:275:LEU:HD12	1:D:300:ASN:HD22	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:401:THR:O	2:F:403:PRO:HD3	1.69	0.92
1:H:35:VAL:HG21	1:H:50:LEU:HD23	1.52	0.92
1:H:78:MET:HB2	1:H:86:GLU:HB2	1.49	0.91
1:D:247:GLN:HE22	4:D:400:NAD:H61A	1.19	0.91
2:I:399:ALA:HA	2:I:408:TYR:HA	1.53	0.91
1:H:72:TRP:CZ3	1:H:339:LEU:HB3	2.06	0.91
1:D:163:MET:HE1	1:E:142:ASN:HD21	1.34	0.91
1:A:264:THR:HG22	1:A:293:LEU:HD12	1.54	0.90
1:A:354:LEU:HD21	1:A:356:MET:CE	2.01	0.90
1:E:125:MET:SD	1:E:126:PRO:HD2	2.12	0.89
1:D:87:VAL:O	1:D:115:ARG:HD3	1.73	0.88
1:H:261:ALA:HB3	1:H:290:ILE:HG13	1.53	0.88
2:C:464:ASN:C	2:C:464:ASN:HD22	1.77	0.88
1:D:322:ASN:HD22	1:D:325:SER:HB2	1.35	0.88
1:B:106:ARG:O	1:B:109:VAL:HG12	1.74	0.88
1:H:122:MET:H	1:H:122:MET:HE2	1.38	0.88
1:H:47:ASP:CB	1:H:57:ILE:CD1	2.51	0.88
1:E:95:VAL:HG12	1:E:118:THR:HB	1.55	0.87
2:F:324:GLN:NE2	2:F:359:LEU:HD22	1.90	0.86
1:H:119:ALA:O	1:H:367:CYS:HA	1.74	0.86
1:D:88:ALA:HA	1:D:115:ARG:HD2	1.57	0.86
1:D:270:LYS:HE2	1:D:270:LYS:HA	1.57	0.86
1:D:342:PHE:O	1:D:345:PRO:HD2	1.75	0.86
1:H:129:SER:HA	1:H:132:GLN:CG	2.05	0.86
1:E:278:GLU:O	1:E:281:VAL:HG12	1.75	0.86
1:H:120:TYR:HA	1:H:366:THR:HG23	1.56	0.86
2:I:399:ALA:HB2	2:I:407:ILE:HG13	1.57	0.86
1:A:289:VAL:HG22	1:A:316:LYS:HB2	1.56	0.86
1:G:72:TRP:HE1	1:G:97:MET:HE1	1.36	0.86
1:H:18:ILE:HD11	1:H:23:VAL:CG2	2.05	0.85
1:D:329:ALA:HB3	1:E:158:ARG:HG3	1.59	0.85
1:H:10:ARG:HH21	1:H:78:MET:HA	1.38	0.85
1:D:21:GLU:CD	2:I:308:SER:HB2	1.97	0.85
1:H:243:PHE:O	1:H:247:GLN:HB3	1.75	0.85
2:C:392:ASN:O	2:C:395:THR:HG22	1.76	0.85
1:H:10:ARG:NH2	1:H:78:MET:HA	1.92	0.85
1:A:105:ASN:O	1:A:108:VAL:HG12	1.76	0.84
1:D:70:VAL:HG12	1:D:95:VAL:HB	1.58	0.84
1:A:265:ALA:HB3	1:A:300:ASN:ND2	1.93	0.84
1:D:175:VAL:HG12	1:D:176:LEU:H	1.43	0.83
1:D:246:LYS:O	1:D:249:GLU:HB3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:367:CYS:SG	1:H:370:ARG:HD3	2.18	0.83
1:A:277:THR:H	1:A:280:MET:CE	1.91	0.83
1:G:376:HIS:O	1:G:380:THR:HG22	1.78	0.83
1:H:136:ILE:HG13	1:H:137:LEU:N	1.93	0.83
1:D:270:LYS:HB3	1:D:271:PRO:HD2	1.60	0.83
1:D:68:ALA:O	1:D:91:LYS:CD	2.27	0.83
1:E:253:LYS:O	1:E:253:LYS:HE3	1.78	0.83
1:E:349:LYS:HG3	1:E:349:LYS:O	1.77	0.82
1:E:90:ILE:HD13	1:E:117:ILE:HD13	1.61	0.82
2:F:432:TYR:CE2	6:F:500:NDP:H6N	2.14	0.82
1:G:158:ARG:HB2	1:H:330:ASP:OD2	1.80	0.82
1:H:93:GLY:HA2	1:H:116:LYS:HB2	1.61	0.82
1:B:340:LEU:O	1:B:344:THR:HG23	1.79	0.82
1:G:256:VAL:HG12	1:G:283:LYS:O	1.79	0.82
1:E:87:VAL:HG23	1:E:112:LEU:HG	1.62	0.81
1:E:358:LEU:H	1:E:358:LEU:HD12	1.43	0.81
1:A:291:ILE:HD13	1:A:318:VAL:HB	1.61	0.81
1:H:61:ALA:HB1	1:H:89:LEU:HD13	1.61	0.81
1:D:239:MET:HB2	1:D:244:ARG:HE	1.44	0.81
1:G:115:ARG:NH2	1:G:115:ARG:HB3	1.96	0.81
1:D:160:PHE:O	1:D:172:PRO:HA	1.81	0.81
2:I:403:PRO:HA	2:I:408:TYR:CG	2.16	0.81
1:D:354:LEU:HD21	1:D:356:MET:SD	2.20	0.81
1:H:136:ILE:HA	1:H:338:ASN:OD1	1.80	0.81
1:H:67:GLN:NE2	1:H:67:GLN:H	1.78	0.81
1:A:58:ALA:HB3	1:A:64:ALA:HB2	1.62	0.81
1:D:5:ILE:HG23	1:D:72:TRP:O	1.81	0.80
1:D:294:ALA:HB3	1:D:300:ASN:OD1	1.81	0.80
1:H:93:GLY:HA2	1:H:116:LYS:CB	2.12	0.80
1:G:10:ARG:HH12	1:G:76:ARG:NH2	1.80	0.80
1:B:8:GLU:CD	1:B:74:VAL:HG22	2.01	0.80
1:G:163:MET:HB2	1:G:170:VAL:CG1	2.11	0.80
1:H:106:ARG:O	1:H:109:VAL:HG12	1.82	0.80
1:D:92:GLU:HB2	1:D:115:ARG:O	1.81	0.79
2:I:451:ASP:OD1	2:I:453:LYS:HB3	1.82	0.79
1:G:221:VAL:HG11	1:G:243:PHE:CZ	2.17	0.79
1:H:67:GLN:HA	1:H:91:LYS:HE3	1.62	0.79
2:C:454:LYS:HE2	2:C:454:LYS:HA	1.65	0.79
1:E:255:LEU:HA	1:E:258:THR:OG1	1.82	0.79
2:I:305:LYS:HE2	2:I:337:GLU:OE1	1.82	0.79
1:D:90:ILE:HD13	1:D:117:ILE:HD13	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:MET:HB2	1:D:170:VAL:CG1	2.13	0.78
1:D:175:VAL:HG21	1:D:191:ALA:HB1	1.63	0.78
1:D:346:HIS:HB3	1:D:355:VAL:O	1.83	0.78
1:H:278:GLU:O	1:H:281:VAL:HG22	1.84	0.78
2:I:336:LYS:HG3	2:I:337:GLU:N	1.97	0.78
1:B:25:LYS:O	1:B:29:LEU:HD13	1.82	0.78
2:I:422:LEU:HG	2:I:448:LEU:HD11	1.66	0.77
1:G:260:ILE:HG12	1:G:289:VAL:HG12	1.66	0.77
1:G:29:LEU:HD11	1:G:344:THR:HG22	1.66	0.77
1:H:362:THR:HG23	1:H:363:VAL:N	2.00	0.77
1:E:278:GLU:HB2	1:E:303:LEU:HD11	1.64	0.77
1:H:340:LEU:HD12	1:H:344:THR:HG23	1.66	0.77
1:B:134:MET:HG2	1:B:342:PHE:N	2.00	0.77
1:H:15:ARG:HH21	1:H:15:ARG:HG2	1.48	0.77
1:B:120:TYR:OH	1:B:356:MET:HG3	1.84	0.77
1:E:177:VAL:HG21	1:E:188:ILE:HD13	1.67	0.77
1:B:123:GLU:HA	1:B:137:LEU:HD11	1.65	0.77
1:G:203:VAL:HG23	1:G:204:ARG:N	2.00	0.77
2:I:451:ASP:HB3	2:I:454:LYS:HG2	1.66	0.77
1:A:163:MET:HB2	1:A:170:VAL:HG13	1.66	0.76
1:H:65:LEU:HD23	1:H:90:ILE:HG23	1.65	0.76
1:B:274:VAL:HG11	1:B:277:THR:HG23	1.67	0.76
2:C:399:ALA:HB2	2:C:407:ILE:CG1	2.15	0.76
1:E:86:GLU:HA	1:E:89:LEU:HD13	1.67	0.76
2:I:401:THR:O	2:I:403:PRO:CD	2.24	0.76
1:D:91:LYS:O	1:D:92:GLU:O	2.03	0.76
1:G:115:ARG:HB3	1:G:115:ARG:HH21	1.50	0.76
1:A:332:SER:HB2	1:A:333:PRO:HD3	1.67	0.76
2:C:330:MET:HG3	2:C:463:MET:HE1	1.66	0.76
2:F:324:GLN:HE21	2:F:359:LEU:HD22	1.49	0.76
1:H:120:TYR:HD2	1:H:366:THR:HG21	1.47	0.76
2:I:316:TYR:O	2:I:320:VAL:HG23	1.86	0.76
1:G:118:THR:HA	1:G:369:THR:O	1.85	0.76
1:E:125:MET:HE2	1:E:134:MET:HB2	1.67	0.76
1:H:100:LEU:HB2	1:H:121:ALA:HB2	1.65	0.76
1:H:112:LEU:HB3	1:H:117:ILE:HG13	1.66	0.76
1:A:376:HIS:HD2	1:A:378:ALA:HB2	1.50	0.75
1:G:170:VAL:HG23	1:H:330:ASP:OD1	1.85	0.75
1:H:113:THR:HG21	1:H:374:ILE:HG13	1.66	0.75
1:D:47:ASP:HA	1:D:50:LEU:HD13	1.69	0.75
1:G:203:VAL:HG23	1:G:204:ARG:H	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:THR:HG22	1:G:293:LEU:HD12	1.68	0.75
1:D:368:VAL:HA	1:D:376:HIS:HB2	1.69	0.75
1:D:291:ILE:N	1:D:291:ILE:HD12	2.02	0.75
2:I:437:ASN:HB3	2:I:440:PHE:HE1	1.49	0.75
1:A:106:ARG:N	1:A:107:PRO:HD2	2.01	0.75
1:D:203:VAL:HG12	1:D:243:PHE:HE2	1.51	0.75
1:D:369:THR:HA	1:D:373:ALA:O	1.87	0.75
1:E:60:THR:CG2	1:E:63:GLN:HG3	2.16	0.75
2:F:354:GLY:O	2:F:358:VAL:HG23	1.86	0.75
1:G:120:TYR:HB3	1:G:366:THR:CG2	2.15	0.75
1:D:3:ILE:O	1:D:33:VAL:HA	1.87	0.74
1:H:142:ASN:HD22	2:I:353:PRO:HD2	1.50	0.74
1:B:369:THR:HB	1:B:374:ILE:HA	1.68	0.74
1:A:165:THR:HG22	2:C:353:PRO:HB3	1.70	0.74
1:A:368:VAL:HA	1:A:376:HIS:HB2	1.69	0.74
1:D:276:ILE:HA	1:D:280:MET:HE3	1.69	0.74
2:F:348:VAL:HG21	2:F:410:MET:HE1	1.69	0.74
2:I:425:LYS:HD3	2:I:427:SER:O	1.88	0.74
2:I:295:GLY:HA3	2:I:446:MET:HE2	1.70	0.73
2:F:328:ARG:HD3	2:F:363:ALA:O	1.88	0.73
1:D:10:ARG:HH21	1:D:10:ARG:HG3	1.52	0.73
2:F:432:TYR:CZ	6:F:500:NDP:H6N	2.23	0.73
1:H:74:VAL:HG23	1:H:75:GLN:N	2.03	0.73
1:H:184:GLY:O	1:H:188:ILE:HG13	1.88	0.73
1:D:157:ALA:O	1:E:329:ALA:HB3	1.89	0.73
1:E:86:GLU:HA	1:E:89:LEU:CD1	2.19	0.73
1:H:118:THR:HA	1:H:369:THR:O	1.89	0.73
1:E:66:SER:O	1:E:91:LYS:HB2	1.89	0.73
1:E:217:LYS:HD2	1:E:217:LYS:N	2.04	0.73
1:D:308:LYS:HG2	1:D:309:ILE:H	1.51	0.73
1:B:113:THR:HG23	1:B:373:ALA:HA	1.70	0.72
1:B:368:VAL:HA	1:B:376:HIS:HB2	1.70	0.72
1:G:2:LYS:HA	1:G:32:GLU:HB2	1.70	0.72
1:H:116:LYS:HA	1:H:372:GLY:N	2.04	0.72
1:D:163:MET:HB2	1:D:170:VAL:HG13	1.71	0.72
1:G:62:ALA:HB2	1:G:89:LEU:HD23	1.71	0.72
1:A:376:HIS:CD2	1:A:378:ALA:HB2	2.24	0.72
1:D:164:MET:HG2	2:F:357:ASN:HD21	1.54	0.72
1:E:244:ARG:HH21	1:E:244:ARG:CB	2.02	0.72
1:H:367:CYS:SG	1:H:370:ARG:CD	2.77	0.72
1:E:341:ASN:O	1:E:345:PRO:HD3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:ALA:O	1:H:89:LEU:HB3	1.90	0.72
2:C:454:LYS:O	2:C:458:GLN:HG3	1.90	0.72
1:H:93:GLY:CA	1:H:116:LYS:HB2	2.20	0.72
1:B:118:THR:HA	1:B:369:THR:O	1.89	0.72
1:D:264:THR:HG22	1:D:293:LEU:HD12	1.72	0.72
1:G:347:VAL:HG12	1:G:348:ASP:O	1.89	0.72
1:H:186:GLN:HA	2:I:352:MET:CE	2.16	0.72
1:D:23:VAL:HG11	1:D:55:ALA:HB2	1.71	0.71
1:A:276:ILE:HA	1:A:280:MET:CE	2.21	0.71
1:B:128:ILE:HD11	1:B:130:ARG:HD3	1.70	0.71
1:E:90:ILE:CD1	1:E:117:ILE:HD13	2.19	0.71
1:G:166:ALA:HB1	1:H:133:SER:HA	1.71	0.71
1:A:278:GLU:HB2	1:A:303:LEU:HD11	1.72	0.71
1:E:312:LYS:HE3	1:E:313:HIS:NE2	2.05	0.71
1:H:180:VAL:HG11	1:H:207:THR:HG23	1.71	0.71
1:B:147:ARG:HD2	1:B:151:ASP:OD2	1.91	0.71
1:D:285:LYS:HD3	1:D:286:PRO:N	2.04	0.71
1:D:293:LEU:CD2	1:D:323:VAL:HG21	2.21	0.71
1:H:32:GLU:HA	1:H:32:GLU:OE2	1.90	0.71
1:H:63:GLN:HA	1:H:63:GLN:HE21	1.56	0.71
2:C:322:GLN:NE2	2:C:324:GLN:HE22	1.89	0.71
1:H:368:VAL:O	1:H:375:VAL:N	2.21	0.71
1:E:244:ARG:HH21	1:E:244:ARG:HB3	1.56	0.71
1:H:93:GLY:HA2	1:H:116:LYS:O	1.90	0.70
1:G:106:ARG:N	1:G:107:PRO:HD2	2.05	0.70
1:G:275:LEU:HB2	1:G:300:ASN:HB3	1.72	0.70
1:H:202:ASP:HA	4:H:400:NAD:H8A	1.71	0.70
1:A:76:ARG:HG2	1:A:76:ARG:NH2	1.97	0.70
1:H:120:TYR:CD2	1:H:366:THR:HG21	2.23	0.70
1:D:207:THR:HA	1:D:210:GLN:HE21	1.56	0.70
1:H:120:TYR:CA	1:H:366:THR:HG23	2.21	0.70
1:B:346:HIS:O	1:B:355:VAL:HG12	1.91	0.70
1:D:120:TYR:HD1	1:D:366:THR:O	1.75	0.70
1:E:25:LYS:O	1:E:29:LEU:HD13	1.92	0.70
1:D:357:LYS:O	1:D:359:GLU:HG3	1.90	0.70
1:B:94:ALA:O	1:B:117:ILE:HG23	1.91	0.70
1:E:5:ILE:HD13	1:E:35:VAL:HG22	1.73	0.70
1:E:93:GLY:HA2	1:E:116:LYS:HD2	1.74	0.70
1:E:125:MET:HE3	1:E:342:PHE:HD2	1.57	0.70
1:D:265:ALA:O	1:D:266:LEU:HD23	1.90	0.70
1:B:3:ILE:HG13	1:B:70:VAL:HG13	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LYS:HD2	1:D:208:LYS:C	2.12	0.70
1:G:330:ASP:OD1	1:H:158:ARG:HD2	1.91	0.69
1:B:164:MET:CE	1:B:164:MET:HA	2.22	0.69
1:E:118:THR:HA	1:E:369:THR:O	1.93	0.69
1:G:243:PHE:C	1:G:245:LYS:H	1.96	0.69
1:D:120:TYR:HB3	1:D:366:THR:HG22	1.73	0.69
1:H:3:ILE:HA	1:H:70:VAL:O	1.92	0.69
1:A:46:THR:O	1:A:49:ALA:HB3	1.92	0.69
1:E:93:GLY:CA	1:E:116:LYS:HD2	2.22	0.69
1:H:8:GLU:HG2	1:H:74:VAL:CG2	2.20	0.69
1:B:70:VAL:HG23	1:B:95:VAL:CB	2.11	0.69
1:D:326:ARG:HH11	1:D:326:ARG:HG2	1.57	0.69
1:D:358:LEU:HD13	1:D:370:ARG:NH2	2.06	0.69
1:H:103:LEU:H	1:H:103:LEU:HD12	1.57	0.69
1:A:120:TYR:HE2	1:A:363:VAL:HG13	1.57	0.69
1:B:99:HIS:HD2	1:B:101:GLY:H	1.39	0.69
1:B:164:MET:HA	1:B:164:MET:HE2	1.74	0.69
1:D:136:ILE:HG22	1:D:338:ASN:HB3	1.73	0.69
1:H:126:PRO:O	1:H:128:ILE:HG12	1.92	0.69
2:I:399:ALA:HB2	2:I:407:ILE:CG1	2.22	0.69
2:F:299:ASP:O	2:F:303:ILE:HG13	1.92	0.69
1:D:163:MET:CE	1:E:142:ASN:HD21	2.05	0.69
1:D:332:SER:HB2	1:D:333:PRO:HD3	1.75	0.69
2:F:403:PRO:HA	2:F:408:TYR:CG	2.27	0.69
1:H:1:MET:HG2	1:H:31:PHE:HA	1.75	0.69
2:I:403:PRO:HG3	2:I:408:TYR:CE1	2.28	0.69
1:E:278:GLU:O	1:E:282:THR:HG23	1.93	0.69
1:B:199:MET:HG3	1:B:217:LYS:O	1.93	0.69
2:C:325:HIS:CE1	2:C:363:ALA:HA	2.27	0.69
1:E:121:ALA:HB1	1:E:123:GLU:OE1	1.93	0.69
1:E:362:THR:HG23	1:E:363:VAL:N	2.06	0.69
1:G:247:GLN:HG2	1:G:248:ALA:N	2.08	0.68
1:H:348:ASP:HB2	1:H:355:VAL:HB	1.75	0.68
1:E:120:TYR:HD1	1:E:366:THR:O	1.75	0.68
1:D:188:ILE:HG12	1:D:198:VAL:HG11	1.75	0.68
1:D:113:THR:HA	1:D:369:THR:HG21	1.76	0.68
1:E:128:ILE:CD1	1:E:130:ARG:HH21	2.07	0.68
1:H:291:ILE:HD12	1:H:291:ILE:N	2.08	0.68
1:E:320:HIS:ND1	1:E:326:ARG:CZ	2.56	0.68
1:G:72:TRP:HE1	1:G:97:MET:CE	2.07	0.68
1:B:6:PRO:HD2	1:B:72:TRP:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:VAL:HA	1:D:326:ARG:HD3	1.76	0.68
1:D:367:CYS:O	1:D:376:HIS:HB2	1.93	0.68
1:E:361:GLU:HA	1:E:364:SER:HB3	1.74	0.68
1:H:178:PHE:HE1	1:H:276:ILE:HD11	1.59	0.68
1:H:210:GLN:O	1:H:213:SER:HB3	1.93	0.68
1:A:7:LYS:HB2	1:A:39:ALA:HA	1.75	0.68
1:B:308:LYS:HG3	1:B:309:ILE:H	1.58	0.68
1:G:121:ALA:HB3	1:G:124:LEU:HD12	1.74	0.68
1:G:368:VAL:HG23	1:G:369:THR:HG22	1.76	0.68
1:D:90:ILE:CD1	1:D:117:ILE:HD13	2.23	0.68
1:G:265:ALA:CB	1:G:275:LEU:HD11	2.24	0.68
1:B:208:LYS:O	1:B:212:GLU:HG3	1.94	0.67
2:I:318:MET:HE3	2:I:324:GLN:H	1.59	0.67
1:D:225:ALA:C	1:D:227:LYS:H	1.97	0.67
1:G:105:ASN:C	1:G:107:PRO:HD2	2.14	0.67
1:G:376:HIS:HD2	1:G:378:ALA:HB2	1.59	0.67
1:H:3:ILE:HG13	1:H:70:VAL:O	1.94	0.67
1:H:8:GLU:CG	1:H:74:VAL:HG22	2.23	0.67
1:B:354:LEU:HD21	1:B:356:MET:HG2	1.76	0.67
2:C:299:ASP:O	2:C:303:ILE:HG13	1.94	0.67
1:D:248:ALA:HA	1:D:251:VAL:HG22	1.76	0.67
1:D:285:LYS:NZ	1:D:286:PRO:HG2	2.10	0.67
1:H:129:SER:HA	1:H:132:GLN:CD	2.14	0.67
1:E:112:LEU:H	1:E:112:LEU:HD12	1.60	0.67
1:G:160:PHE:O	1:G:172:PRO:HA	1.95	0.67
1:B:370:ARG:HG2	1:B:375:VAL:HG21	1.76	0.67
2:F:312:ILE:HG21	2:F:327:LEU:HD21	1.77	0.67
1:H:158:ARG:HB3	1:H:158:ARG:HH11	1.60	0.67
1:A:265:ALA:HB3	1:A:300:ASN:HD21	1.58	0.67
2:C:396:ASN:O	2:C:412:ILE:HD13	1.94	0.67
1:D:78:MET:HA	1:D:82:GLU:OE1	1.94	0.67
1:D:342:PHE:HZ	1:D:362:THR:O	1.73	0.67
1:H:266:LEU:O	1:H:267:ILE:HG13	1.95	0.67
1:A:164:MET:HE3	2:C:357:ASN:OD1	1.95	0.67
1:B:244:ARG:H	1:B:244:ARG:HD3	1.60	0.67
1:D:354:LEU:HD23	1:D:355:VAL:N	2.10	0.67
1:E:97:MET:O	1:E:98:CYS:HB3	1.95	0.67
1:G:265:ALA:HB3	1:G:275:LEU:HD11	1.77	0.67
1:B:217:LYS:HA	1:B:217:LYS:HE3	1.75	0.67
1:E:113:THR:HG23	1:E:373:ALA:HA	1.75	0.67
1:G:278:GLU:O	1:G:282:THR:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:GLN:HE21	1:H:248:ALA:N	1.93	0.67
2:F:381:GLN:HG2	2:F:417:LYS:HE2	1.76	0.66
1:B:108:VAL:O	1:B:112:LEU:HD13	1.94	0.66
1:G:78:MET:H	1:G:86:GLU:HB2	1.59	0.66
1:G:263:THR:OG1	1:G:292:ASP:HA	1.95	0.66
1:H:69:ASP:O	1:H:95:VAL:HG23	1.95	0.66
1:H:110:GLU:HA	1:H:374:ILE:HD11	1.77	0.66
1:H:218:PHE:HD2	1:H:220:THR:HG23	1.59	0.66
2:C:310:VAL:HG22	2:C:385:VAL:HB	1.77	0.66
1:B:349:LYS:HG3	1:B:350:ASP:N	2.07	0.66
1:E:204:ARG:O	1:E:207:THR:HB	1.96	0.66
1:H:182:VAL:HG13	1:H:183:ALA:N	2.11	0.66
1:H:284:MET:SD	1:H:290:ILE:HD11	2.36	0.66
2:C:309:LYS:NZ	2:C:382:THR:HB	2.11	0.66
1:G:362:THR:CG2	1:G:363:VAL:N	2.59	0.66
2:I:318:MET:HG3	2:I:319:ALA:N	2.11	0.66
1:A:277:THR:H	1:A:280:MET:HE2	1.60	0.66
1:G:359:GLU:CD	1:G:359:GLU:H	1.99	0.66
1:H:264:THR:HG22	1:H:293:LEU:HD12	1.78	0.66
1:A:93:GLY:HA2	1:A:116:LYS:O	1.95	0.66
1:D:20:PRO:HD3	1:D:45:ILE:HG21	1.78	0.66
1:E:284:MET:HE1	1:E:315:VAL:HG11	1.77	0.66
2:F:446:MET:HE3	2:F:448:LEU:HD21	1.78	0.66
1:H:346:HIS:HB3	1:H:356:MET:HB3	1.78	0.66
2:F:388:VAL:HG13	2:F:391:ALA:HB3	1.78	0.66
1:D:70:VAL:HA	1:D:95:VAL:O	1.96	0.66
1:D:167:ALA:O	1:E:337:LYS:HD2	1.96	0.66
1:D:96:LEU:HD23	1:D:96:LEU:O	1.96	0.65
1:E:60:THR:HG22	1:E:63:GLN:HG3	1.76	0.65
1:G:362:THR:HG22	1:G:363:VAL:N	2.11	0.65
1:H:178:PHE:CE1	1:H:276:ILE:HD11	2.30	0.65
1:B:267:ILE:CD1	4:B:400:NAD:N1A	2.59	0.65
1:D:87:VAL:O	1:D:115:ARG:CD	2.44	0.65
2:C:433:ALA:O	2:C:435:VAL:HG23	1.96	0.65
1:D:354:LEU:C	1:D:355:VAL:HG22	2.16	0.65
1:G:113:THR:HG23	1:G:373:ALA:HA	1.78	0.65
1:B:136:ILE:HA	1:B:338:ASN:OD1	1.97	0.65
1:H:355:VAL:HG13	1:H:355:VAL:O	1.95	0.65
1:D:50:LEU:H	1:D:50:LEU:HD12	1.61	0.65
1:D:277:THR:H	1:D:280:MET:HE3	1.62	0.65
1:H:136:ILE:HG13	1:H:137:LEU:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:401:THR:C	2:I:403:PRO:HD3	2.15	0.65
1:D:322:ASN:ND2	1:D:325:SER:HB2	2.11	0.65
1:H:5:ILE:HB	1:H:35:VAL:HG12	1.79	0.65
1:G:120:TYR:OH	1:G:356:MET:HG3	1.97	0.65
1:H:7:LYS:HB2	1:H:39:ALA:HA	1.79	0.65
1:A:167:ALA:HB2	1:B:338:ASN:HD21	1.62	0.65
1:B:136:ILE:HG13	1:B:137:LEU:HD12	1.77	0.65
1:G:89:LEU:HD12	1:G:89:LEU:H	1.60	0.65
1:G:362:THR:HG22	1:G:363:VAL:H	1.61	0.65
1:A:136:ILE:HG13	1:A:137:LEU:N	2.12	0.65
1:D:97:MET:HB2	1:D:122:MET:CE	2.27	0.65
1:G:5:ILE:HB	1:G:35:VAL:HG12	1.79	0.65
2:F:304:MET:HG2	2:F:385:VAL:HG11	1.79	0.64
2:I:432:TYR:C	2:I:434:GLY:H	1.98	0.64
2:F:454:LYS:HA	2:F:457:GLU:OE1	1.96	0.64
1:H:295:VAL:HG23	1:H:304:SER:HB2	1.79	0.64
2:I:437:ASN:HB3	2:I:440:PHE:CD1	2.32	0.64
2:C:420:THR:HB	1:H:162:MET:CE	2.28	0.64
1:D:57:ILE:HD12	1:D:58:ALA:H	1.61	0.64
1:G:103:LEU:HD13	1:G:124:LEU:HD21	1.78	0.64
1:H:281:VAL:HG11	1:H:303:LEU:HD12	1.79	0.64
1:D:88:ALA:HA	1:D:115:ARG:CD	2.27	0.64
1:H:5:ILE:HG13	1:H:72:TRP:CD1	2.33	0.64
1:H:247:GLN:NE2	1:H:248:ALA:N	2.45	0.64
1:B:143:LEU:HD12	1:B:331:ALA:HB2	1.78	0.64
1:E:128:ILE:HD11	1:E:130:ARG:HH21	1.63	0.64
1:H:208:LYS:NZ	1:H:220:THR:HG21	2.12	0.64
1:H:241:GLU:O	1:H:245:LYS:HG2	1.97	0.64
1:B:10:ARG:HH11	1:B:10:ARG:HG3	1.62	0.64
1:B:29:LEU:CD2	1:B:347:VAL:HG11	2.21	0.64
1:G:67:GLN:HA	1:G:91:LYS:HD3	1.80	0.64
1:H:162:MET:HB2	1:H:172:PRO:HD3	1.80	0.64
1:A:304:SER:O	1:A:305:GLU:C	2.36	0.64
1:G:66:SER:O	1:G:91:LYS:HB3	1.98	0.64
1:A:207:THR:HG22	1:A:218:PHE:HE1	1.63	0.64
1:D:329:ALA:HB3	1:E:157:ALA:O	1.98	0.64
1:G:94:ALA:O	1:G:117:ILE:HG23	1.98	0.64
1:B:180:VAL:HG23	1:B:202:ASP:HB2	1.79	0.64
2:F:366:PRO:HB2	2:F:369:GLU:HG3	1.80	0.63
1:G:273:PRO:HG3	4:G:400:NAD:H2A	1.80	0.63
1:A:6:PRO:HA	1:A:36:GLU:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PRO:HG2	1:B:362:THR:HA	1.80	0.63
1:B:264:THR:CG2	1:B:293:LEU:HD12	2.20	0.63
1:D:246:LYS:O	1:D:249:GLU:CB	2.46	0.63
1:D:346:HIS:CD2	1:D:356:MET:HA	2.34	0.63
1:B:376:HIS:HB3	1:B:379:LEU:HD13	1.80	0.63
1:D:106:ARG:O	1:D:109:VAL:HG22	1.98	0.63
1:E:136:ILE:CD1	1:E:137:LEU:HD12	2.28	0.63
1:A:375:VAL:HG22	1:A:375:VAL:O	1.98	0.63
1:B:19:SER:HB3	1:B:22:VAL:HG23	1.80	0.63
1:D:263:THR:OG1	1:D:292:ASP:HA	1.97	0.63
1:A:180:VAL:HG11	1:A:207:THR:HG23	1.80	0.63
1:G:120:TYR:CE2	1:G:363:VAL:HG13	2.33	0.63
1:B:86:GLU:O	1:B:89:LEU:HB2	1.98	0.63
2:C:430:SER:OG	2:C:434:GLY:HA2	1.99	0.63
1:E:374:ILE:H	1:E:374:ILE:HD12	1.63	0.63
1:G:282:THR:HG22	1:G:313:HIS:HD2	1.64	0.63
1:E:362:THR:CG2	1:E:363:VAL:N	2.60	0.63
1:H:122:MET:H	1:H:122:MET:CE	2.12	0.63
2:I:410:MET:HG3	2:I:410:MET:O	1.99	0.63
1:A:276:ILE:HA	1:A:280:MET:HE3	1.81	0.63
1:A:376:HIS:HD2	1:A:378:ALA:CB	2.12	0.63
2:C:424:ILE:O	2:C:424:ILE:HG22	1.99	0.63
1:D:3:ILE:HB	1:D:70:VAL:HG23	1.81	0.63
1:E:89:LEU:H	1:E:89:LEU:HD12	1.64	0.63
1:B:5:ILE:HD12	1:B:5:ILE:N	2.14	0.62
1:E:34:ILE:CD1	1:E:56:THR:HB	2.28	0.62
1:H:120:TYR:HB3	1:H:366:THR:HG21	1.80	0.62
1:A:120:TYR:CE2	1:A:363:VAL:HG13	2.34	0.62
1:D:121:ALA:O	1:D:124:LEU:HB2	1.99	0.62
1:B:147:ARG:CD	1:B:151:ASP:OD2	2.47	0.62
1:D:2:LYS:HD2	1:D:32:GLU:HB3	1.81	0.62
1:D:277:THR:H	1:D:280:MET:CE	2.12	0.62
1:E:86:GLU:C	1:E:88:ALA:H	2.03	0.62
1:G:5:ILE:HD12	1:G:5:ILE:N	2.14	0.62
2:F:344:ALA:HB2	2:F:376:ILE:HD13	1.82	0.62
1:H:272:ALA:HB1	1:H:273:PRO:HD2	1.80	0.62
1:D:163:MET:HE1	1:E:142:ASN:ND2	2.11	0.62
1:H:362:THR:CG2	1:H:363:VAL:H	2.07	0.62
2:I:377:ASN:O	2:I:379:SER:N	2.31	0.62
1:H:276:ILE:O	1:H:302:PRO:HD2	1.99	0.62
1:D:178:PHE:CE2	1:D:276:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:O	1:B:256:VAL:HG23	2.00	0.61
1:A:342:PHE:CE1	1:A:362:THR:HG23	2.34	0.61
1:D:194:LEU:HD21	1:E:194:LEU:HD13	1.82	0.61
1:E:60:THR:HG22	1:E:63:GLN:CG	2.29	0.61
1:E:348:ASP:CG	1:E:351:THR:HB	2.20	0.61
2:I:323:ALA:O	2:I:325:HIS:N	2.34	0.61
2:C:395:THR:HG23	2:C:437:ASN:HD21	1.64	0.61
1:H:60:THR:HG23	1:H:63:GLN:H	1.63	0.61
2:I:330:MET:HG3	2:I:463:MET:HE3	1.82	0.61
1:A:163:MET:HB2	1:A:170:VAL:CG1	2.29	0.61
1:A:322:ASN:ND2	1:A:325:SER:HB2	2.14	0.61
1:B:274:VAL:CG1	1:B:277:THR:HG23	2.31	0.61
2:C:316:TYR:O	2:C:320:VAL:HG23	2.00	0.61
2:C:403:PRO:HA	2:C:408:TYR:CG	2.34	0.61
2:C:464:ASN:C	2:C:464:ASN:ND2	2.48	0.61
1:D:3:ILE:HG13	1:D:70:VAL:O	2.01	0.61
1:G:243:PHE:O	1:G:247:GLN:HB3	2.00	0.61
1:G:257:LYS:HA	1:G:285:LYS:HE3	1.82	0.61
1:B:96:LEU:HD23	1:B:112:LEU:HD21	1.82	0.61
1:E:16:VAL:HG22	1:E:18:ILE:HG22	1.82	0.61
1:G:326:ARG:HG2	1:G:326:ARG:HH21	1.66	0.61
1:G:376:HIS:HD2	1:G:378:ALA:CB	2.13	0.61
1:H:34:ILE:HG23	1:H:58:ALA:HB2	1.82	0.61
2:I:437:ASN:CB	2:I:440:PHE:HE1	2.13	0.61
1:D:92:GLU:H	1:D:115:ARG:HH21	1.47	0.61
1:D:120:TYR:CD1	1:D:366:THR:O	2.54	0.61
1:D:136:ILE:HD13	1:D:137:LEU:N	2.16	0.61
1:D:366:THR:O	1:D:366:THR:HG22	1.99	0.61
1:E:93:GLY:N	1:E:116:LYS:O	2.32	0.61
2:F:451:ASP:H	2:F:454:LYS:HE3	1.65	0.61
1:H:321:THR:O	1:H:322:ASN:HB2	2.00	0.61
1:B:1:MET:CE	1:B:353:THR:HA	2.30	0.61
1:D:5:ILE:HG12	1:D:18:ILE:HB	1.82	0.61
1:G:36:GLU:OE1	1:G:61:ALA:HB2	2.01	0.61
1:A:45:ILE:HG22	1:A:50:LEU:HD21	1.81	0.61
1:B:190:THR:O	1:B:193:ARG:HG2	2.00	0.61
1:G:139:SER:HB2	1:G:334:LEU:HD23	1.82	0.61
1:G:374:ILE:HD12	1:G:374:ILE:H	1.66	0.61
1:H:2:LYS:HD3	1:H:32:GLU:HB2	1.82	0.61
2:I:308:SER:HB3	2:I:384:ASP:OD2	2.00	0.61
2:F:310:VAL:HG22	2:F:385:VAL:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:ALA:C	1:H:65:LEU:HD12	2.21	0.61
1:B:19:SER:O	1:B:23:VAL:HG23	1.99	0.61
1:B:22:VAL:HG21	1:B:336:ALA:HB1	1.83	0.61
1:D:285:LYS:HD3	1:D:285:LYS:C	2.22	0.61
1:H:120:TYR:CB	1:H:366:THR:CG2	2.79	0.61
1:H:208:LYS:HZ2	1:H:220:THR:HG21	1.66	0.61
1:E:342:PHE:CD1	1:E:342:PHE:O	2.54	0.60
2:I:403:PRO:HA	2:I:408:TYR:CD2	2.35	0.60
2:C:424:ILE:N	2:C:424:ILE:HD12	2.16	0.60
1:E:169:THR:HG22	1:E:170:VAL:N	2.16	0.60
1:B:312:LYS:HG2	1:B:313:HIS:CD2	2.36	0.60
2:C:403:PRO:HA	2:C:408:TYR:CD1	2.36	0.60
1:E:34:ILE:HD13	1:E:56:THR:HB	1.81	0.60
1:D:76:ARG:HG2	1:D:100:LEU:HA	1.83	0.60
1:D:131:ALA:HB1	1:D:134:MET:HG3	1.83	0.60
1:D:97:MET:HB2	1:D:122:MET:HE1	1.84	0.60
1:E:125:MET:HE3	1:E:134:MET:SD	2.42	0.60
1:E:360:ASP:CG	1:E:362:THR:HG22	2.21	0.60
1:G:9:ARG:NH2	1:G:36:GLU:OE2	2.34	0.60
1:G:221:VAL:HG12	1:G:222:ASP:N	2.16	0.60
1:H:47:ASP:HB2	1:H:57:ILE:CD1	2.32	0.60
1:H:70:VAL:HA	1:H:95:VAL:HB	1.83	0.60
1:H:112:LEU:HD12	1:H:112:LEU:N	2.15	0.60
1:H:163:MET:HB2	1:H:170:VAL:HG23	1.83	0.60
1:A:141:SER:O	1:A:183:ALA:HB2	2.01	0.60
1:B:120:TYR:CE1	1:B:367:CYS:HB2	2.36	0.60
2:C:303:ILE:HG12	1:H:169:THR:CG2	2.31	0.60
1:D:50:LEU:O	1:D:55:ALA:HB3	2.02	0.60
1:E:284:MET:CE	1:E:290:ILE:HD11	2.32	0.60
1:A:376:HIS:CD2	1:A:378:ALA:H	2.19	0.60
2:C:373:LEU:HD23	2:C:373:LEU:C	2.22	0.60
1:D:158:ARG:HG3	1:E:329:ALA:HB3	1.84	0.60
1:B:118:THR:HG23	1:B:370:ARG:HB3	1.83	0.60
1:D:91:LYS:O	1:D:92:GLU:C	2.40	0.60
1:D:265:ALA:HB3	1:D:300:ASN:HD21	1.67	0.60
2:I:453:LYS:O	2:I:457:GLU:HG3	2.01	0.60
1:D:68:ALA:H	1:D:91:LYS:HD2	1.67	0.60
1:G:104:THR:O	1:G:104:THR:HG22	2.02	0.60
2:C:321:ALA:CB	2:C:452:ALA:HB3	2.31	0.59
1:D:342:PHE:CE1	1:D:362:THR:HG23	2.37	0.59
1:E:138:SER:OG	1:E:139:SER:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:ARG:HG2	1:G:75:GLN:HG2	1.83	0.59
1:G:115:ARG:HH21	1:G:115:ARG:CB	2.13	0.59
1:G:311:VAL:HG13	1:G:316:LYS:HG2	1.83	0.59
1:H:87:VAL:HG21	1:H:112:LEU:HA	1.83	0.59
1:A:277:THR:H	1:A:280:MET:HE3	1.65	0.59
1:B:146:TYR:CE2	1:B:150:ILE:HG13	2.37	0.59
1:H:5:ILE:HG13	1:H:72:TRP:HD1	1.68	0.59
1:H:28:GLY:C	1:H:29:LEU:HD12	2.22	0.59
1:H:278:GLU:O	1:H:282:THR:HG23	2.02	0.59
1:A:13:GLU:OE2	1:A:15:ARG:HB2	2.02	0.59
1:B:99:HIS:CD2	1:B:101:GLY:H	2.19	0.59
1:G:2:LYS:O	1:G:69:ASP:HB2	2.03	0.59
1:G:374:ILE:HD12	1:G:374:ILE:N	2.17	0.59
1:H:142:ASN:ND2	2:I:353:PRO:HB2	2.17	0.59
1:H:147:ARG:NH1	1:H:151:ASP:OD1	2.35	0.59
1:A:106:ARG:HH12	1:A:379:LEU:HG	1.65	0.59
1:D:280:MET:C	1:D:282:THR:H	2.05	0.59
1:G:128:ILE:HD12	1:G:129:SER:H	1.67	0.59
1:H:131:ALA:HA	1:H:134:MET:CE	2.32	0.59
1:H:162:MET:HE2	1:H:164:MET:SD	2.42	0.59
1:D:13:GLU:OE1	1:D:322:ASN:ND2	2.36	0.59
1:D:221:VAL:HG11	1:D:250:ALA:HB3	1.82	0.59
1:H:4:ALA:O	1:H:71:VAL:HG23	2.03	0.59
1:E:219:ILE:O	1:E:219:ILE:HG22	2.02	0.59
1:G:34:ILE:HD13	1:G:56:THR:HB	1.83	0.59
1:G:37:GLN:NE2	1:G:59:SER:HA	2.17	0.59
1:G:78:MET:HA	1:G:82:GLU:OE1	2.02	0.59
1:H:18:ILE:CD1	1:H:23:VAL:HG22	2.16	0.59
1:H:47:ASP:HB2	1:H:57:ILE:HD13	1.80	0.59
1:D:5:ILE:HD12	1:D:5:ILE:N	2.18	0.59
1:H:72:TRP:HA	1:H:97:MET:O	2.02	0.59
1:H:347:VAL:C	1:H:355:VAL:HG12	2.23	0.59
1:B:7:LYS:HG3	1:B:39:ALA:HA	1.85	0.59
2:F:407:ILE:HG13	2:F:408:TYR:N	2.18	0.59
1:H:15:ARG:HB2	1:H:332:SER:OG	2.02	0.59
1:G:5:ILE:HG12	1:G:18:ILE:HB	1.85	0.59
1:H:7:LYS:HB2	1:H:39:ALA:CB	2.33	0.59
1:A:58:ALA:CB	1:A:64:ALA:HB2	2.33	0.59
1:E:60:THR:HG23	1:E:63:GLN:H	1.67	0.59
2:F:437:ASN:C	2:F:439:LEU:H	2.06	0.59
2:I:346:HIS:CD2	2:I:394:VAL:HB	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ALA:HA	1:A:134:MET:HE2	1.83	0.58
1:H:67:GLN:HA	1:H:91:LYS:CE	2.32	0.58
2:C:346:HIS:HD2	2:C:373:LEU:HD12	1.69	0.58
1:D:73:LYS:O	1:D:98:CYS:CB	2.45	0.58
1:D:252:LEU:O	1:D:256:VAL:HG13	2.03	0.58
1:D:360:ASP:OD2	1:D:362:THR:HB	2.04	0.58
1:E:76:ARG:HD2	1:E:108:VAL:HG21	1.85	0.58
1:G:120:TYR:HE2	1:G:363:VAL:HG13	1.67	0.58
1:G:374:ILE:H	1:G:374:ILE:CD1	2.17	0.58
1:B:73:LYS:HZ1	1:B:77:PRO:HD3	1.66	0.58
1:H:7:LYS:HD2	1:H:38:GLY:O	2.03	0.58
1:H:163:MET:HB2	1:H:170:VAL:CG2	2.34	0.58
1:A:131:ALA:HA	1:A:134:MET:CE	2.33	0.58
1:D:125:MET:HE3	1:D:134:MET:HB2	1.85	0.58
1:E:89:LEU:HD12	1:E:89:LEU:N	2.18	0.58
1:G:309:ILE:HG23	1:G:318:VAL:HG22	1.84	0.58
1:H:63:GLN:HA	1:H:63:GLN:NE2	2.19	0.58
1:D:25:LYS:HB3	1:D:340:LEU:HD11	1.84	0.58
1:D:106:ARG:HB2	1:D:107:PRO:HD3	1.84	0.58
1:D:237:LYS:HA	1:D:267:ILE:HG23	1.86	0.58
1:H:60:THR:O	1:H:64:ALA:HB3	2.04	0.58
1:D:106:ARG:H	1:D:106:ARG:HD2	1.67	0.58
1:D:308:LYS:HD2	1:D:309:ILE:O	2.04	0.58
1:H:125:MET:HA	1:H:125:MET:CE	2.34	0.58
1:B:66:SER:HB2	1:B:67:GLN:OE1	2.04	0.58
1:H:113:THR:O	1:H:372:GLY:HA2	2.03	0.58
1:B:188:ILE:HG23	1:B:198:VAL:HG11	1.86	0.58
1:D:99:HIS:CE1	1:D:123:GLU:HB3	2.39	0.58
1:E:176:LEU:HD23	1:E:199:MET:O	2.02	0.58
2:F:446:MET:CE	2:F:448:LEU:HD21	2.32	0.58
1:H:120:TYR:CG	1:H:366:THR:CG2	2.86	0.58
1:E:202:ASP:OD2	1:E:203:VAL:N	2.36	0.57
1:G:10:ARG:NH1	1:G:76:ARG:CZ	2.67	0.57
1:E:86:GLU:O	1:E:88:ALA:N	2.37	0.57
1:E:374:ILE:HD12	1:E:374:ILE:N	2.19	0.57
1:H:142:ASN:ND2	2:I:353:PRO:HD2	2.18	0.57
2:I:325:HIS:CE1	2:I:363:ALA:HA	2.39	0.57
2:C:371:PHE:HB2	2:C:376:ILE:HG12	1.85	0.57
1:D:293:LEU:HD21	1:D:323:VAL:HG21	1.86	0.57
1:E:106:ARG:HB3	1:E:107:PRO:HD3	1.86	0.57
1:E:183:ALA:HB3	1:E:264:THR:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:313:VAL:HB	2:I:388:VAL:HG22	1.86	0.57
1:B:100:LEU:C	1:B:102:ALA:N	2.55	0.57
1:D:357:LYS:O	1:D:359:GLU:N	2.37	0.57
1:G:180:VAL:HG21	1:G:211:VAL:HG21	1.86	0.57
1:H:67:GLN:H	1:H:67:GLN:CD	2.07	0.57
1:H:124:LEU:HD13	1:H:365:GLY:O	2.04	0.57
1:D:179:GLY:HA2	4:D:400:NAD:H8A	1.85	0.57
1:E:183:ALA:HB3	1:E:264:THR:HG21	1.85	0.57
1:G:10:ARG:NH1	1:G:76:ARG:NH2	2.51	0.57
1:G:34:ILE:CD1	1:G:56:THR:HB	2.34	0.57
1:G:160:PHE:N	1:G:161:PRO:HD2	2.19	0.57
1:B:136:ILE:HG13	1:B:137:LEU:N	2.18	0.57
1:D:60:THR:OG1	1:D:63:GLN:HG2	2.05	0.57
1:D:329:ALA:CB	1:E:158:ARG:HG3	2.33	0.57
1:E:16:VAL:O	1:E:18:ILE:N	2.38	0.57
1:H:16:VAL:HG22	1:H:17:ALA:H	1.69	0.57
1:H:309:ILE:HG12	1:H:318:VAL:HG13	1.85	0.57
1:B:67:GLN:HG2	1:B:67:GLN:O	2.05	0.57
1:D:151:ASP:CG	1:D:326:ARG:HH21	2.08	0.57
1:G:273:PRO:HG3	4:G:400:NAD:C2A	2.34	0.57
1:A:97:MET:HE3	1:A:343:LEU:HD12	1.85	0.57
1:D:4:ALA:HB1	1:D:34:ILE:O	2.04	0.57
1:E:127:ARG:NH2	1:E:132:GLN:HG3	2.20	0.57
1:E:370:ARG:HH21	1:E:375:VAL:HG11	1.70	0.57
2:F:373:LEU:HD23	2:F:373:LEU:C	2.24	0.57
1:G:282:THR:HG22	1:G:313:HIS:CD2	2.39	0.57
1:B:242:GLU:O	1:B:245:LYS:HB3	2.05	0.57
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.20	0.57
1:H:346:HIS:NE2	1:H:362:THR:HG21	2.20	0.57
1:A:69:ASP:O	1:A:95:VAL:HG23	2.05	0.57
1:B:18:ILE:HG12	1:B:19:SER:N	2.19	0.57
1:B:62:ALA:HA	1:B:89:LEU:HD22	1.87	0.57
2:C:414:ASP:HB3	2:C:417:LYS:HE3	1.87	0.57
1:D:221:VAL:CG1	1:D:250:ALA:HB3	2.34	0.57
2:F:437:ASN:HB3	2:F:440:PHE:CE2	2.40	0.57
1:H:202:ASP:CG	4:H:400:NAD:H8A	2.25	0.57
1:E:136:ILE:HD12	1:E:137:LEU:HD12	1.87	0.56
1:E:199:MET:CG	1:E:219:ILE:HD11	2.28	0.56
1:H:282:THR:HG22	1:H:313:HIS:CD2	2.39	0.56
1:B:5:ILE:HG13	1:B:72:TRP:HB2	1.87	0.56
1:B:266:LEU:H	4:B:400:NAD:H52A	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ASP:HB2	1:D:227:LYS:HE2	1.86	0.56
1:G:200:ALA:HB3	1:G:211:VAL:HG11	1.88	0.56
1:G:243:PHE:O	1:G:245:LYS:N	2.38	0.56
1:H:2:LYS:O	1:H:69:ASP:HB2	2.04	0.56
2:I:310:VAL:HG22	2:I:385:VAL:HB	1.86	0.56
1:A:178:PHE:HB3	1:A:275:LEU:HD13	1.87	0.56
1:A:276:ILE:HA	1:A:280:MET:HE1	1.87	0.56
1:D:175:VAL:HG12	1:D:176:LEU:N	2.17	0.56
1:E:125:MET:CE	1:E:134:MET:HB2	2.34	0.56
2:F:450:GLY:HA3	2:F:455:MET:CE	2.35	0.56
1:H:70:VAL:HG23	1:H:95:VAL:HB	1.87	0.56
1:H:243:PHE:C	1:H:245:LYS:H	2.08	0.56
1:H:312:LYS:HG3	1:H:313:HIS:CD2	2.40	0.56
2:I:302:PHE:O	2:I:306:ASN:HB2	2.06	0.56
2:I:380:PHE:HZ	2:I:413:LEU:HD22	1.70	0.56
2:I:439:LEU:C	2:I:441:PHE:H	2.08	0.56
2:I:440:PHE:HD2	2:I:447:MET:SD	2.28	0.56
1:A:80:ALA:HA	1:A:85:ASP:HB2	1.87	0.56
1:B:96:LEU:HD23	1:B:112:LEU:CD2	2.36	0.56
1:D:50:LEU:C	1:D:55:ALA:HB3	2.25	0.56
1:E:143:LEU:HD12	1:E:331:ALA:HB2	1.86	0.56
1:E:250:ALA:O	1:E:253:LYS:HB3	2.05	0.56
1:H:73:LYS:HD2	1:H:75:GLN:O	2.05	0.56
2:I:304:MET:C	2:I:306:ASN:H	2.05	0.56
1:B:137:LEU:HD12	1:B:137:LEU:H	1.71	0.56
1:B:190:THR:HA	1:B:193:ARG:HD2	1.87	0.56
1:D:208:LYS:HD2	1:D:209:GLU:N	2.20	0.56
1:D:281:VAL:O	1:D:281:VAL:HG12	2.04	0.56
1:E:264:THR:O	1:E:264:THR:HG22	2.04	0.56
1:E:362:THR:CG2	1:E:363:VAL:H	2.18	0.56
1:G:118:THR:CB	1:G:370:ARG:HA	2.35	0.56
1:H:124:LEU:O	1:H:125:MET:C	2.44	0.56
1:D:35:VAL:HG21	1:D:50:LEU:HD23	1.87	0.56
1:D:351:THR:O	1:D:353:THR:HG22	2.06	0.56
1:E:128:ILE:O	1:E:128:ILE:HG13	2.04	0.56
1:G:199:MET:CE	1:G:217:LYS:HB2	2.35	0.56
1:H:116:LYS:HA	1:H:372:GLY:H	1.69	0.56
1:H:265:ALA:HB3	1:H:300:ASN:OD1	2.04	0.56
1:B:73:LYS:HZ1	1:B:77:PRO:CD	2.18	0.56
2:C:303:ILE:HG12	1:H:169:THR:HG21	1.87	0.56
1:D:342:PHE:CE1	1:D:362:THR:O	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:LYS:HB2	1:E:39:ALA:CB	2.36	0.56
1:E:160:PHE:CZ	1:E:260:ILE:HD12	2.40	0.56
1:G:342:PHE:HE1	1:G:362:THR:HG23	1.71	0.56
1:H:179:GLY:O	1:H:181:GLY:N	2.39	0.56
1:H:182:VAL:HG13	1:H:183:ALA:H	1.70	0.56
1:B:354:LEU:HD11	1:B:356:MET:SD	2.46	0.56
1:D:68:ALA:O	1:D:91:LYS:CG	2.54	0.56
1:G:274:VAL:HG13	1:G:302:PRO:HD3	1.88	0.56
1:H:202:ASP:HA	4:H:400:NAD:C8A	2.35	0.56
2:I:393:ASP:OD1	2:I:431:GLY:HA3	2.05	0.56
1:D:285:LYS:HZ1	1:E:44:SER:HB3	1.70	0.56
1:G:281:VAL:O	1:G:281:VAL:HG12	2.06	0.56
2:I:452:ALA:H	6:I:500:NDP:C2A	2.19	0.56
1:B:66:SER:O	1:B:91:LYS:HB2	2.06	0.56
1:B:87:VAL:HG13	1:B:88:ALA:N	2.21	0.56
1:D:221:VAL:HG21	1:D:247:GLN:HA	1.88	0.56
2:F:410:MET:HG3	2:F:411:PRO:HD2	1.88	0.56
1:H:72:TRP:CE3	1:H:339:LEU:HB3	2.40	0.56
1:A:270:LYS:CB	1:A:271:PRO:CD	2.78	0.55
1:B:291:ILE:HD13	1:B:318:VAL:HB	1.88	0.55
1:D:2:LYS:HD2	1:D:32:GLU:CB	2.35	0.55
1:G:180:VAL:HG12	1:G:185:LEU:HG	1.89	0.55
1:G:255:LEU:HD21	1:G:276:ILE:HD11	1.87	0.55
1:H:18:ILE:HG12	1:H:19:SER:N	2.21	0.55
2:I:451:ASP:O	2:I:452:ALA:C	2.44	0.55
2:C:346:HIS:CD2	2:C:373:LEU:HD12	2.41	0.55
1:G:164:MET:HE1	2:I:370:VAL:HG12	1.88	0.55
1:G:164:MET:CE	2:I:370:VAL:HG12	2.36	0.55
2:I:298:GLU:N	2:I:298:GLU:OE2	2.37	0.55
1:A:2:LYS:HB3	1:A:68:ALA:HA	1.88	0.55
1:D:24:LYS:NZ	1:D:24:LYS:HB3	2.21	0.55
1:G:344:THR:OG1	1:G:345:PRO:HD3	2.06	0.55
1:H:74:VAL:CG2	1:H:75:GLN:H	2.12	0.55
1:G:376:HIS:CD2	1:G:378:ALA:HB2	2.40	0.55
1:H:47:ASP:CB	1:H:57:ILE:HD11	2.35	0.55
1:H:295:VAL:O	1:H:295:VAL:HG22	2.06	0.55
1:A:149:VAL:HG11	1:A:190:THR:HG22	1.89	0.55
1:B:76:ARG:HB3	1:B:100:LEU:HA	1.88	0.55
1:H:92:GLU:HB2	1:H:116:LYS:NZ	2.21	0.55
1:B:120:TYR:HB3	1:B:366:THR:HG21	1.88	0.55
1:H:33:VAL:O	1:H:34:ILE:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:GLY:O	1:H:185:LEU:HD12	2.06	0.55
2:F:455:MET:O	2:F:459:ILE:HG13	2.06	0.55
1:D:223:ASP:HB3	1:D:228:THR:HG21	1.89	0.55
1:E:2:LYS:HD3	1:E:32:GLU:CB	2.36	0.55
1:G:326:ARG:HG2	1:G:326:ARG:NH2	2.22	0.55
1:G:326:ARG:O	3:O:2:FRU:O4	2.25	0.55
1:H:156:PHE:CE2	1:H:158:ARG:HB2	2.41	0.55
1:A:194:LEU:HD21	1:B:194:LEU:HG	1.88	0.55
1:D:26:LEU:HD11	1:D:72:TRP:CZ3	2.42	0.55
1:D:34:ILE:HG23	1:D:56:THR:O	2.07	0.55
1:G:106:ARG:N	1:G:107:PRO:CD	2.69	0.55
1:G:111:ALA:HA	1:G:114:LYS:HG3	1.88	0.55
1:H:8:GLU:H	1:H:8:GLU:CD	2.09	0.55
1:E:108:VAL:O	1:E:112:LEU:HD12	2.07	0.55
1:G:280:MET:C	1:G:282:THR:H	2.10	0.55
1:E:284:MET:HE2	1:E:290:ILE:HD11	1.89	0.54
1:G:23:VAL:HG11	1:G:55:ALA:HB2	1.89	0.54
2:C:315:GLY:HA3	2:C:391:ALA:HB2	1.89	0.54
1:D:18:ILE:HD13	1:D:18:ILE:C	2.28	0.54
1:D:29:LEU:HD22	1:D:347:VAL:HG11	1.90	0.54
1:D:344:THR:HA	1:D:347:VAL:HG23	1.88	0.54
1:D:357:LYS:C	1:D:359:GLU:H	2.10	0.54
1:E:9:ARG:O	1:E:10:ARG:C	2.45	0.54
2:I:305:LYS:HB2	2:I:337:GLU:OE1	2.06	0.54
2:I:323:ALA:O	2:I:326:ALA:N	2.35	0.54
2:I:371:PHE:HB2	2:I:376:ILE:HB	1.89	0.54
2:I:403:PRO:HG3	2:I:408:TYR:CZ	2.42	0.54
1:A:375:VAL:O	1:A:375:VAL:CG2	2.55	0.54
2:C:324:GLN:HB2	2:C:363:ALA:HB2	1.89	0.54
1:D:32:GLU:O	1:D:34:ILE:HD12	2.07	0.54
1:E:1:MET:CG	1:E:352:LYS:O	2.55	0.54
1:G:180:VAL:HG21	1:G:211:VAL:CG2	2.36	0.54
1:G:182:VAL:HG12	4:G:400:NAD:O1N	2.07	0.54
1:H:8:GLU:HG3	1:H:73:LYS:HE2	1.89	0.54
1:H:25:LYS:HA	1:H:25:LYS:CE	2.37	0.54
1:H:277:THR:OG1	1:H:280:MET:HG3	2.08	0.54
2:I:422:LEU:HD12	2:I:446:MET:HB3	1.88	0.54
2:C:399:ALA:HA	2:C:408:TYR:HA	1.90	0.54
1:H:15:ARG:HH21	1:H:15:ARG:CG	2.19	0.54
1:H:300:ASN:HD22	1:H:300:ASN:N	2.06	0.54
2:I:330:MET:HG3	2:I:463:MET:CE	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG21	1:A:207:THR:HG21	1.88	0.54
1:A:277:THR:O	1:A:279:GLU:N	2.41	0.54
1:A:380:THR:O	1:A:380:THR:HG22	2.08	0.54
1:B:118:THR:HA	1:B:370:ARG:HA	1.90	0.54
1:D:2:LYS:NZ	1:D:32:GLU:HG2	2.23	0.54
1:D:164:MET:HG3	2:F:345:ILE:HG21	1.89	0.54
1:D:205:ALA:C	1:D:207:THR:H	2.11	0.54
1:E:303:LEU:H	1:E:303:LEU:HD12	1.73	0.54
1:H:202:ASP:CB	1:H:207:THR:HG21	2.38	0.54
2:I:422:LEU:HG	2:I:448:LEU:CD1	2.35	0.54
1:A:147:ARG:HG3	1:A:151:ASP:OD2	2.07	0.54
1:B:370:ARG:HH12	1:B:375:VAL:HG11	1.72	0.54
1:D:10:ARG:HG3	1:D:10:ARG:NH2	2.21	0.54
1:D:164:MET:HG2	2:F:357:ASN:ND2	2.22	0.54
1:E:121:ALA:HB1	1:E:123:GLU:CD	2.28	0.54
1:A:21:GLU:H	1:A:21:GLU:CD	2.10	0.54
1:D:4:ALA:HB2	1:D:34:ILE:HB	1.90	0.54
1:D:294:ALA:O	1:D:299:GLY:N	2.41	0.54
1:A:97:MET:CE	1:A:343:LEU:HD12	2.38	0.54
2:C:330:MET:HG2	2:C:334:LEU:CD2	2.38	0.54
1:D:193:ARG:HB3	1:E:193:ARG:O	2.07	0.54
2:I:309:LYS:O	2:I:384:ASP:HB2	2.08	0.54
1:E:177:VAL:CG2	1:E:188:ILE:HD13	2.38	0.54
1:H:291:ILE:HD12	1:H:291:ILE:H	1.73	0.54
1:A:360:ASP:OD2	1:A:362:THR:HB	2.08	0.54
1:B:5:ILE:HG23	1:B:17:ALA:HB3	1.89	0.54
1:B:204:ARG:HH21	1:B:207:THR:HG22	1.73	0.54
1:B:379:LEU:HD12	1:B:379:LEU:N	2.23	0.54
2:C:321:ALA:O	2:C:322:GLN:HB2	2.08	0.54
1:D:270:LYS:HB3	1:D:271:PRO:CD	2.36	0.54
1:E:78:MET:HG3	1:E:86:GLU:OE1	2.08	0.54
1:E:369:THR:O	1:E:369:THR:HG23	2.06	0.54
2:F:348:VAL:HG21	2:F:410:MET:CE	2.37	0.54
1:A:80:ALA:CA	1:A:85:ASP:HB2	2.38	0.53
1:A:354:LEU:HD11	1:A:356:MET:HE1	1.90	0.53
1:B:128:ILE:HG12	1:B:131:ALA:CB	2.37	0.53
1:B:244:ARG:HA	1:B:247:GLN:HB3	1.90	0.53
1:G:62:ALA:HB2	1:G:89:LEU:CD2	2.37	0.53
1:H:203:VAL:HG12	1:H:243:PHE:CZ	2.44	0.53
1:B:199:MET:HE2	1:B:217:LYS:HB3	1.89	0.53
1:E:86:GLU:C	1:E:88:ALA:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:VAL:O	1:E:111:ALA:HB3	2.08	0.53
1:H:7:LYS:HB2	1:H:39:ALA:CA	2.38	0.53
2:I:395:THR:HB	2:I:415:VAL:HG21	1.89	0.53
1:A:140:GLN:C	1:A:142:ASN:H	2.11	0.53
1:B:106:ARG:HB3	1:B:107:PRO:HD3	1.90	0.53
2:C:379:SER:O	2:C:382:THR:N	2.41	0.53
1:D:164:MET:CG	2:F:357:ASN:HD21	2.21	0.53
1:E:58:ALA:CB	1:E:64:ALA:HA	2.38	0.53
1:H:214:LEU:HD11	2:I:352:MET:SD	2.49	0.53
1:B:100:LEU:O	1:B:102:ALA:N	2.42	0.53
2:C:321:ALA:HB3	2:C:452:ALA:HB3	1.90	0.53
1:A:4:ALA:HB1	1:A:64:ALA:O	2.08	0.53
1:B:120:TYR:HB3	1:B:366:THR:CG2	2.39	0.53
1:B:137:LEU:HD12	1:B:137:LEU:N	2.24	0.53
1:D:293:LEU:HD23	1:D:323:VAL:HG21	1.91	0.53
1:G:284:MET:HG3	1:G:315:VAL:HG21	1.90	0.53
1:A:265:ALA:CB	1:A:275:LEU:HD11	2.39	0.53
1:D:6:PRO:HD2	1:D:72:TRP:O	2.08	0.53
1:E:5:ILE:N	1:E:5:ILE:HD12	2.24	0.53
1:G:62:ALA:CA	1:G:89:LEU:HD23	2.38	0.53
1:H:7:LYS:O	1:H:9:ARG:HD2	2.09	0.53
1:H:112:LEU:N	1:H:112:LEU:CD1	2.71	0.53
1:A:113:THR:HG22	1:A:114:LYS:N	2.24	0.53
1:A:327:VAL:HG12	1:A:327:VAL:O	2.08	0.53
1:B:190:THR:HA	1:B:193:ARG:CD	2.39	0.53
1:D:8:GLU:HB3	1:D:13:GLU:HB3	1.91	0.53
1:E:344:THR:O	1:E:347:VAL:HG12	2.08	0.53
2:F:346:HIS:HB3	2:F:349:ALA:HB2	1.90	0.53
1:G:95:VAL:HG22	1:G:118:THR:HG23	1.90	0.53
1:G:203:VAL:CG2	1:G:204:ARG:H	2.18	0.53
1:H:38:GLY:H	1:H:47:ASP:CG	2.12	0.53
1:H:203:VAL:H	4:H:400:NAD:C8A	2.21	0.53
1:H:263:THR:OG1	1:H:292:ASP:HA	2.08	0.53
1:H:295:VAL:CG2	1:H:304:SER:HB2	2.39	0.53
2:I:463:MET:O	2:I:464:ASN:HB2	2.09	0.53
1:A:327:VAL:HG12	1:A:330:ASP:HB2	1.91	0.53
2:C:420:THR:HB	1:H:162:MET:HE1	1.91	0.53
1:D:202:ASP:OD1	1:D:203:VAL:N	2.41	0.53
1:E:214:LEU:HD21	2:F:355:HIS:CD2	2.44	0.53
2:F:374:GLU:H	2:F:374:GLU:CD	2.11	0.53
1:G:62:ALA:CB	1:G:89:LEU:HD23	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:ILE:HD12	1:G:129:SER:N	2.23	0.53
1:D:123:GLU:HG2	1:D:124:LEU:HD13	1.89	0.53
2:F:445:THR:HG22	2:F:446:MET:N	2.24	0.53
1:G:22:VAL:HG13	1:G:340:LEU:HD12	1.91	0.53
2:I:331:ALA:O	2:I:335:LYS:HD3	2.09	0.53
1:B:71:VAL:HG12	1:B:96:LEU:HA	1.90	0.53
1:B:100:LEU:C	1:B:102:ALA:H	2.13	0.53
1:B:272:ALA:HB1	1:B:300:ASN:HD21	1.74	0.53
2:C:392:ASN:HB3	6:C:500:NDP:O1A	2.09	0.53
1:D:8:GLU:OE1	1:D:75:GLN:N	2.40	0.53
1:D:122:MET:C	1:D:124:LEU:H	2.11	0.53
1:D:244:ARG:N	1:D:244:ARG:HD3	2.24	0.53
1:E:80:ALA:HA	1:E:85:ASP:HB2	1.91	0.53
1:G:194:LEU:HD11	1:H:194:LEU:HG	1.91	0.53
1:H:176:LEU:HA	1:H:199:MET:O	2.09	0.53
2:I:451:ASP:H	2:I:454:LYS:HE2	1.73	0.53
1:A:277:THR:N	1:A:280:MET:HE3	2.24	0.52
1:B:5:ILE:HD13	1:B:18:ILE:HD12	1.91	0.52
1:B:265:ALA:HB3	1:B:275:LEU:HD11	1.90	0.52
1:D:267:ILE:O	1:D:268:PRO:O	2.27	0.52
1:E:3:ILE:O	1:E:3:ILE:HG23	2.08	0.52
2:F:416:GLU:HG3	2:F:439:LEU:HD11	1.91	0.52
1:G:153:ALA:HA	1:G:160:PHE:CE1	2.44	0.52
1:B:1:MET:HE2	1:B:353:THR:HA	1.91	0.52
1:E:2:LYS:HD3	1:E:32:GLU:HB2	1.90	0.52
1:E:312:LYS:O	1:E:313:HIS:HB2	2.09	0.52
1:G:78:MET:N	1:G:86:GLU:HB2	2.23	0.52
2:C:455:MET:O	2:C:459:ILE:HG13	2.10	0.52
1:D:105:ASN:O	1:D:108:VAL:HG12	2.09	0.52
1:E:178:PHE:CE1	1:E:276:ILE:HD11	2.44	0.52
1:G:177:VAL:HG11	1:G:188:ILE:HG12	1.91	0.52
1:H:85:ASP:OD2	1:H:88:ALA:HB3	2.09	0.52
1:H:103:LEU:HD12	1:H:103:LEU:N	2.23	0.52
1:H:330:ASP:C	1:H:333:PRO:HD2	2.29	0.52
1:B:273:PRO:HG3	4:B:400:NAD:N6A	2.24	0.52
1:D:3:ILE:HG22	1:D:31:PHE:HB3	1.90	0.52
1:D:265:ALA:HB3	1:D:300:ASN:ND2	2.24	0.52
1:D:327:VAL:O	1:D:329:ALA:N	2.43	0.52
1:D:342:PHE:C	1:D:345:PRO:HD2	2.29	0.52
1:H:294:ALA:C	1:H:296:GLU:H	2.12	0.52
1:B:73:LYS:HZ1	1:B:77:PRO:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:LYS:HG2	1:D:309:ILE:N	2.23	0.52
1:E:136:ILE:HD12	1:E:136:ILE:C	2.30	0.52
1:E:252:LEU:O	1:E:256:VAL:HG22	2.10	0.52
2:F:374:GLU:OE1	2:F:374:GLU:N	2.42	0.52
1:H:122:MET:C	1:H:124:LEU:H	2.13	0.52
1:B:278:GLU:O	1:B:281:VAL:HG22	2.10	0.52
1:E:58:ALA:HB3	1:E:64:ALA:HB2	1.90	0.52
1:E:180:VAL:O	1:E:180:VAL:HG12	2.09	0.52
1:E:291:ILE:HD13	1:E:318:VAL:HB	1.91	0.52
2:F:450:GLY:HA3	2:F:455:MET:HE3	1.92	0.52
1:G:370:ARG:O	1:G:371:ASP:C	2.46	0.52
1:A:46:THR:HG23	1:A:49:ALA:CB	2.30	0.52
1:A:85:ASP:OD2	1:A:88:ALA:HB2	2.09	0.52
2:C:456:THR:O	2:C:460:VAL:HG23	2.10	0.52
1:E:264:THR:CG2	1:E:264:THR:O	2.57	0.52
1:H:277:THR:O	1:H:281:VAL:HG13	2.10	0.52
1:H:340:LEU:CD1	1:H:344:THR:HG23	2.38	0.52
2:I:319:ALA:HA	2:I:359:LEU:HD13	1.92	0.52
2:I:333:VAL:O	2:I:336:LYS:HG2	2.09	0.52
1:A:207:THR:HG22	1:A:218:PHE:CE1	2.42	0.52
1:A:355:VAL:O	1:A:355:VAL:HG13	2.10	0.52
1:B:78:MET:HG3	1:B:86:GLU:OE1	2.10	0.52
1:B:368:VAL:CG1	1:B:379:LEU:HD22	2.40	0.52
1:E:260:ILE:HG12	1:E:289:VAL:CG1	2.40	0.52
2:F:459:ILE:O	2:F:463:MET:HG3	2.10	0.52
1:G:7:LYS:HG3	1:G:39:ALA:HA	1.92	0.52
1:H:98:CYS:N	1:H:122:MET:HE1	2.25	0.52
2:I:324:GLN:HG2	2:I:325:HIS:H	1.75	0.52
1:A:275:LEU:O	1:A:280:MET:HE1	2.10	0.52
1:A:370:ARG:HD2	1:A:375:VAL:HG11	1.92	0.52
2:C:346:HIS:CD2	2:C:347:PRO:HD2	2.45	0.52
1:D:18:ILE:HD12	1:D:50:LEU:HD23	1.90	0.52
1:D:203:VAL:HG23	1:D:204:ARG:HG3	1.90	0.52
1:E:22:VAL:HG13	1:E:340:LEU:HD22	1.92	0.52
1:E:72:TRP:NE1	1:E:97:MET:CE	2.73	0.52
1:H:147:ARG:HG3	1:H:327:VAL:HG22	1.92	0.52
1:H:203:VAL:HG23	1:H:204:ARG:H	1.75	0.52
1:H:203:VAL:HG23	1:H:204:ARG:N	2.24	0.52
1:B:184:GLY:O	1:B:187:ALA:HB3	2.10	0.52
1:B:242:GLU:HA	1:B:242:GLU:OE2	2.10	0.52
2:C:309:LYS:HZ1	2:C:382:THR:HB	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:VAL:HB	1:D:324:PRO:HD3	1.92	0.52
1:E:207:THR:HG22	1:E:218:PHE:CE2	2.44	0.52
1:G:132:GLN:HG2	4:G:400:NAD:O7N	2.10	0.52
2:I:336:LYS:HG3	2:I:337:GLU:H	1.75	0.52
2:I:453:LYS:HE2	2:I:457:GLU:CD	2.31	0.52
1:A:115:ARG:O	1:A:116:LYS:HB2	2.10	0.51
1:A:262:ILE:HD13	1:A:291:ILE:HB	1.91	0.51
1:A:277:THR:C	1:A:279:GLU:N	2.64	0.51
1:A:305:GLU:HB3	1:A:308:LYS:HD2	1.92	0.51
1:A:374:ILE:HB	1:A:380:THR:HG21	1.92	0.51
1:B:370:ARG:NH1	1:B:375:VAL:HG11	2.24	0.51
1:E:120:TYR:OH	1:E:356:MET:HG3	2.10	0.51
2:F:424:ILE:O	2:F:424:ILE:HG22	2.09	0.51
1:H:37:GLN:HA	1:H:57:ILE:CG2	2.40	0.51
1:H:180:VAL:O	1:H:180:VAL:HG12	2.10	0.51
2:I:317:GLY:HA3	2:I:390:GLY:HA3	1.92	0.51
1:D:282:THR:O	1:D:282:THR:HG22	2.11	0.51
1:E:320:HIS:CE1	1:E:326:ARG:NH2	2.79	0.51
1:G:203:VAL:CG2	1:G:204:ARG:N	2.69	0.51
1:A:80:ALA:HB2	1:A:85:ASP:HB2	1.91	0.51
1:A:222:ASP:OD2	1:A:222:ASP:N	2.44	0.51
1:B:339:LEU:O	1:B:341:ASN:N	2.44	0.51
1:D:68:ALA:N	1:D:91:LYS:HD2	2.25	0.51
1:E:252:LEU:O	1:E:252:LEU:HG	2.08	0.51
2:F:407:ILE:O	2:F:408:TYR:C	2.49	0.51
1:G:208:LYS:O	1:G:212:GLU:HG3	2.09	0.51
1:H:96:LEU:C	1:H:96:LEU:HD23	2.30	0.51
1:H:103:LEU:HD11	1:H:124:LEU:HD21	1.91	0.51
1:H:125:MET:HA	1:H:125:MET:HE2	1.92	0.51
1:H:128:ILE:O	1:H:132:GLN:CG	2.58	0.51
2:I:304:MET:C	2:I:306:ASN:N	2.63	0.51
2:I:380:PHE:CZ	2:I:413:LEU:HD22	2.44	0.51
2:I:432:TYR:C	2:I:434:GLY:N	2.64	0.51
1:D:3:ILE:CB	1:D:70:VAL:HG23	2.41	0.51
1:D:7:LYS:O	1:D:9:ARG:HG3	2.11	0.51
1:D:285:LYS:NZ	1:E:44:SER:HB3	2.26	0.51
1:E:19:SER:O	1:E:23:VAL:HG23	2.09	0.51
1:E:125:MET:CE	1:E:342:PHE:HD2	2.20	0.51
1:B:244:ARG:H	1:B:244:ARG:CD	2.24	0.51
1:E:266:LEU:HD13	1:E:294:ALA:HA	1.92	0.51
1:G:176:LEU:HD23	1:G:199:MET:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:VAL:HG12	1:A:212:GLU:N	2.25	0.51
1:D:89:LEU:O	1:D:89:LEU:HD23	2.11	0.51
1:D:248:ALA:HA	1:D:251:VAL:CG2	2.40	0.51
1:D:267:ILE:HD11	4:D:400:NAD:H2A	1.93	0.51
2:F:432:TYR:CD2	6:F:500:NDP:C1D	2.84	0.51
1:H:202:ASP:CA	4:H:400:NAD:H8A	2.39	0.51
1:H:266:LEU:HD12	1:H:272:ALA:HB2	1.92	0.51
1:H:368:VAL:HG13	1:H:376:HIS:HB3	1.93	0.51
2:I:445:THR:HG22	2:I:447:MET:HE2	1.93	0.51
1:B:73:LYS:NZ	1:B:75:GLN:O	2.38	0.51
1:B:275:LEU:HG	1:B:300:ASN:HB3	1.93	0.51
1:D:91:LYS:O	1:D:91:LYS:HG3	2.11	0.51
1:D:160:PHE:N	1:D:161:PRO:HD2	2.26	0.51
1:D:275:LEU:CD1	1:D:300:ASN:HD22	2.13	0.51
1:E:60:THR:HG22	1:E:63:GLN:HB2	1.93	0.51
1:E:136:ILE:HA	1:E:338:ASN:OD1	2.10	0.51
1:G:13:GLU:OE2	1:G:15:ARG:HB2	2.11	0.51
1:G:113:THR:CG2	1:G:373:ALA:HA	2.41	0.51
1:G:133:SER:O	1:G:338:ASN:HA	2.11	0.51
1:H:120:TYR:HB3	1:H:366:THR:CG2	2.40	0.51
1:H:128:ILE:HG12	1:H:131:ALA:HB3	1.93	0.51
1:A:160:PHE:O	1:A:172:PRO:HA	2.11	0.51
2:C:309:LYS:HZ3	2:C:382:THR:HB	1.76	0.51
1:D:136:ILE:HG22	1:D:338:ASN:CB	2.39	0.51
1:D:304:SER:O	1:D:305:GLU:HG2	2.11	0.51
2:F:412:ILE:O	2:F:412:ILE:HD12	2.11	0.51
1:G:23:VAL:HG13	1:G:33:VAL:HG11	1.93	0.51
1:G:23:VAL:CG1	1:G:55:ALA:HB2	2.40	0.51
1:G:154:TYR:O	1:H:147:ARG:NH2	2.36	0.51
1:H:182:VAL:CG1	1:H:183:ALA:N	2.74	0.51
1:H:266:LEU:HD13	1:H:294:ALA:HB2	1.92	0.51
2:I:336:LYS:CG	2:I:337:GLU:N	2.72	0.51
1:A:17:ALA:HB2	1:A:74:VAL:HG22	1.92	0.51
1:E:7:LYS:HB2	1:E:39:ALA:HA	1.92	0.51
1:H:61:ALA:O	1:H:65:LEU:HD22	2.11	0.51
1:H:112:LEU:O	1:H:115:ARG:HB2	2.11	0.51
2:I:389:ILE:HG23	2:I:389:ILE:O	2.10	0.51
1:B:22:VAL:HG21	1:B:336:ALA:CB	2.41	0.50
1:B:74:VAL:HG23	1:B:75:GLN:N	2.26	0.50
1:B:188:ILE:HA	1:B:198:VAL:HG11	1.93	0.50
1:B:281:VAL:HA	1:B:284:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:413:LEU:O	2:C:415:VAL:N	2.43	0.50
1:D:267:ILE:O	1:D:267:ILE:HG22	2.10	0.50
1:E:270:LYS:N	1:E:270:LYS:HE3	2.26	0.50
2:F:432:TYR:HD2	6:F:500:NDP:H1D	1.68	0.50
1:G:128:ILE:O	1:G:130:ARG:N	2.44	0.50
1:H:29:LEU:CD2	1:H:344:THR:HG22	2.41	0.50
1:H:129:SER:C	1:H:132:GLN:HG3	2.31	0.50
1:H:357:LYS:HB3	1:H:360:ASP:CB	2.34	0.50
2:I:433:ALA:C	2:I:435:VAL:H	2.14	0.50
1:A:273:PRO:O	1:A:300:ASN:HA	2.10	0.50
1:B:3:ILE:HG13	1:B:70:VAL:CG1	2.41	0.50
1:B:98:CYS:SG	1:B:100:LEU:HG	2.52	0.50
1:E:212:GLU:C	1:E:214:LEU:N	2.63	0.50
1:E:279:GLU:O	1:E:282:THR:OG1	2.20	0.50
1:H:65:LEU:HD12	1:H:65:LEU:N	2.26	0.50
2:I:324:GLN:HG2	2:I:325:HIS:N	2.26	0.50
1:A:313:HIS:O	1:A:315:VAL:HG23	2.11	0.50
1:D:5:ILE:N	1:D:34:ILE:O	2.41	0.50
1:D:7:LYS:HB2	1:D:39:ALA:HA	1.92	0.50
1:D:16:VAL:HG11	1:D:40:GLY:HA3	1.91	0.50
1:D:252:LEU:C	1:D:254:GLU:H	2.13	0.50
1:G:22:VAL:HG13	1:G:340:LEU:CD1	2.41	0.50
1:G:89:LEU:HD12	1:G:89:LEU:N	2.26	0.50
1:G:158:ARG:HD3	1:H:330:ASP:OD2	2.10	0.50
1:H:3:ILE:CG2	1:H:33:VAL:HG22	2.41	0.50
1:H:179:GLY:HA3	1:H:264:THR:OG1	2.12	0.50
2:I:328:ARG:HD2	2:I:328:ARG:O	2.11	0.50
1:D:5:ILE:O	1:D:35:VAL:HA	2.11	0.50
1:D:23:VAL:O	1:D:26:LEU:N	2.42	0.50
1:D:97:MET:HB2	1:D:122:MET:HE2	1.94	0.50
1:D:291:ILE:N	1:D:291:ILE:CD1	2.74	0.50
1:E:176:LEU:HA	1:E:199:MET:O	2.12	0.50
1:B:5:ILE:HB	1:B:35:VAL:HG12	1.94	0.50
1:D:74:VAL:HG12	1:D:75:GLN:N	2.26	0.50
1:D:343:LEU:HG	1:D:354:LEU:HD12	1.93	0.50
1:B:134:MET:HG2	1:B:342:PHE:H	1.75	0.50
1:B:176:LEU:HA	1:B:199:MET:O	2.12	0.50
1:D:23:VAL:CG1	1:D:55:ALA:HB2	2.39	0.50
1:D:68:ALA:C	1:D:91:LYS:HD3	2.29	0.50
1:D:285:LYS:HD3	1:D:286:PRO:CD	2.42	0.50
1:E:266:LEU:CD1	1:E:294:ALA:HA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:ILE:H	1:E:374:ILE:CD1	2.24	0.50
1:G:86:GLU:HA	1:G:89:LEU:HD13	1.92	0.50
1:G:199:MET:HE1	1:G:217:LYS:HB2	1.93	0.50
1:G:208:LYS:NZ	1:G:220:THR:HG23	2.27	0.50
1:G:299:GLY:C	1:G:301:CYS:H	2.15	0.50
1:H:180:VAL:HG21	1:H:211:VAL:CG2	2.41	0.50
1:D:252:LEU:C	1:D:252:LEU:HD23	2.32	0.50
1:D:294:ALA:CB	1:D:300:ASN:OD1	2.58	0.50
1:D:376:HIS:CD2	1:D:378:ALA:HB2	2.46	0.50
1:E:105:ASN:O	1:E:109:VAL:HG23	2.12	0.50
1:G:78:MET:H	1:G:86:GLU:CB	2.24	0.50
1:G:97:MET:HE1	1:G:343:LEU:HD13	1.93	0.50
1:H:103:LEU:H	1:H:103:LEU:CD1	2.23	0.50
1:H:182:VAL:CG1	1:H:183:ALA:H	2.25	0.50
1:H:297:ALA:C	1:H:299:GLY:H	2.15	0.50
1:B:29:LEU:HD21	1:B:344:THR:HB	1.93	0.50
1:D:191:ALA:O	1:D:196:ALA:HB3	2.12	0.50
1:E:120:TYR:CD1	1:E:366:THR:O	2.61	0.50
1:H:243:PHE:O	1:H:245:LYS:N	2.40	0.50
1:E:282:THR:HG22	1:E:313:HIS:CE1	2.47	0.50
1:H:113:THR:HG23	1:H:369:THR:OG1	2.12	0.50
1:H:311:VAL:HG23	1:H:315:VAL:O	2.12	0.50
1:H:360:ASP:O	1:H:362:THR:N	2.45	0.50
1:A:74:VAL:HA	1:A:335:PHE:CE2	2.47	0.49
1:D:78:MET:HB2	1:D:86:GLU:HG3	1.92	0.49
1:E:172:PRO:HG3	2:I:443:ASN:O	2.12	0.49
2:F:437:ASN:HB3	2:F:440:PHE:CZ	2.47	0.49
1:G:380:THR:HG23	1:G:380:THR:O	2.12	0.49
1:B:156:PHE:CZ	1:B:259:ASP:HB3	2.47	0.49
1:D:46:THR:O	1:D:50:LEU:HD12	2.12	0.49
1:E:360:ASP:OD1	1:E:362:THR:HG22	2.12	0.49
1:G:160:PHE:CZ	1:G:260:ILE:HD12	2.47	0.49
1:G:291:ILE:HG22	1:G:291:ILE:O	2.10	0.49
1:H:58:ALA:CB	1:H:64:ALA:HA	2.42	0.49
1:D:360:ASP:CG	1:D:362:THR:HB	2.33	0.49
1:E:366:THR:O	1:E:366:THR:HG22	2.11	0.49
1:G:158:ARG:HB2	1:H:330:ASP:HB2	1.95	0.49
1:G:360:ASP:OD1	1:G:362:THR:HB	2.12	0.49
1:H:113:THR:HG22	1:H:372:GLY:O	2.13	0.49
1:H:244:ARG:HE	1:H:247:GLN:HE22	1.59	0.49
1:A:223:ASP:OD2	1:A:243:PHE:HZ	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:SD	1:D:353:THR:HA	2.52	0.49
1:E:180:VAL:HG11	1:E:211:VAL:HG22	1.95	0.49
1:E:272:ALA:CB	1:E:299:GLY:H	2.25	0.49
2:I:337:GLU:O	2:I:337:GLU:HG3	2.13	0.49
1:B:18:ILE:HG12	1:B:19:SER:H	1.77	0.49
1:E:128:ILE:HD11	1:E:130:ARG:NH2	2.26	0.49
1:E:200:ALA:O	1:E:219:ILE:HG12	2.12	0.49
1:E:370:ARG:HB2	1:E:375:VAL:HG21	1.94	0.49
1:H:266:LEU:HD12	1:H:272:ALA:CB	2.42	0.49
1:H:292:ASP:HB3	1:H:295:VAL:HB	1.94	0.49
1:B:344:THR:HA	1:B:347:VAL:HG12	1.95	0.49
1:D:199:MET:CG	1:D:219:ILE:HD11	2.43	0.49
1:D:334:LEU:HD22	1:E:167:ALA:CB	2.43	0.49
1:G:57:ILE:O	1:G:57:ILE:HG22	2.11	0.49
1:H:51:THR:HG23	1:H:55:ALA:O	2.13	0.49
1:H:61:ALA:C	1:H:65:LEU:HD13	2.32	0.49
1:H:135:ASP:OD2	1:H:135:ASP:C	2.50	0.49
1:A:22:VAL:HG13	1:A:340:LEU:HD22	1.94	0.49
1:A:163:MET:HE3	1:A:170:VAL:HG11	1.95	0.49
1:A:184:GLY:O	1:A:188:ILE:HG13	2.13	0.49
1:A:295:VAL:HG13	1:A:296:GLU:N	2.28	0.49
1:A:354:LEU:HG	1:A:355:VAL:N	2.28	0.49
1:B:178:PHE:HB3	1:B:275:LEU:HD13	1.95	0.49
1:B:343:LEU:HD23	1:B:344:THR:N	2.28	0.49
2:F:401:THR:O	2:F:403:PRO:CD	2.52	0.49
1:G:248:ALA:HB1	1:G:280:MET:CE	2.42	0.49
1:B:100:LEU:HD12	1:B:121:ALA:HA	1.95	0.49
1:B:181:GLY:HA3	4:B:400:NAD:O1N	2.13	0.49
2:C:350:GLY:C	6:C:500:NDP:H71N	2.16	0.49
1:D:95:VAL:HG22	1:D:118:THR:HB	1.93	0.49
1:D:118:THR:HG23	1:D:370:ARG:HG3	1.95	0.49
1:D:224:GLU:H	1:D:227:LYS:HG2	1.78	0.49
1:D:330:ASP:CG	1:E:158:ARG:HG2	2.33	0.49
1:D:344:THR:HA	1:D:347:VAL:CG2	2.43	0.49
1:E:164:MET:SD	2:I:446:MET:HE1	2.53	0.49
1:G:10:ARG:NH2	1:G:78:MET:HG3	2.27	0.49
1:H:115:ARG:O	1:H:116:LYS:HB2	2.13	0.49
1:H:348:ASP:N	1:H:353:THR:O	2.43	0.49
1:H:357:LYS:C	1:H:359:GLU:H	2.16	0.49
1:B:339:LEU:O	1:B:340:LEU:C	2.50	0.49
1:D:343:LEU:HD23	1:D:343:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:LEU:O	1:G:31:PHE:HB2	2.12	0.49
1:G:72:TRP:NE1	1:G:97:MET:HE1	2.17	0.49
1:G:73:LYS:HE3	1:G:75:GLN:O	2.13	0.49
2:I:451:ASP:O	2:I:454:LYS:N	2.45	0.49
1:A:103:LEU:HD21	1:A:124:LEU:HD11	1.94	0.49
1:A:265:ALA:HB2	1:A:275:LEU:HD11	1.95	0.49
1:B:19:SER:HB3	1:B:22:VAL:CG2	2.42	0.49
1:G:244:ARG:HG2	1:G:244:ARG:O	2.13	0.49
1:H:25:LYS:HA	1:H:25:LYS:HE3	1.94	0.49
1:H:119:ALA:H	1:H:369:THR:CG2	2.26	0.49
2:I:402:ASP:O	2:I:408:TYR:HB2	2.13	0.49
1:B:128:ILE:HG12	1:B:131:ALA:HB3	1.95	0.48
1:E:122:MET:CE	1:E:339:LEU:HG	2.43	0.48
2:F:305:LYS:HZ2	2:F:337:GLU:HG3	1.77	0.48
1:G:279:GLU:O	1:G:283:LYS:HG2	2.13	0.48
1:H:97:MET:SD	1:H:342:PHE:HE1	2.36	0.48
1:H:178:PHE:CD2	1:H:275:LEU:HD13	2.48	0.48
1:A:17:ALA:HB2	1:A:74:VAL:CG2	2.43	0.48
1:A:305:GLU:HB2	1:A:310:VAL:HG21	1.96	0.48
1:A:363:VAL:O	1:A:363:VAL:HG12	2.13	0.48
1:B:113:THR:HG23	1:B:372:GLY:O	2.14	0.48
1:D:97:MET:O	1:D:98:CYS:HB3	2.13	0.48
1:D:105:ASN:O	1:D:109:VAL:HG13	2.13	0.48
1:D:108:VAL:HG13	1:D:109:VAL:N	2.27	0.48
1:G:130:ARG:NH1	1:G:360:ASP:OD1	2.45	0.48
2:I:435:VAL:HG22	2:I:436:GLU:N	2.28	0.48
1:A:80:ALA:CB	1:A:85:ASP:HB2	2.42	0.48
1:A:163:MET:CE	1:A:170:VAL:HG11	2.43	0.48
1:A:362:THR:HG22	1:A:363:VAL:N	2.28	0.48
1:B:341:ASN:O	1:B:343:LEU:N	2.45	0.48
2:C:392:ASN:O	2:C:395:THR:CG2	2.57	0.48
2:C:395:THR:HG21	2:C:423:PHE:HE2	1.78	0.48
1:D:311:VAL:HA	1:D:315:VAL:O	2.13	0.48
1:D:354:LEU:HD23	1:D:354:LEU:C	2.32	0.48
1:E:10:ARG:NH2	1:E:76:ARG:HG3	2.27	0.48
1:E:169:THR:OG1	2:I:303:ILE:HG12	2.12	0.48
2:F:407:ILE:O	2:F:408:TYR:O	2.31	0.48
1:H:27:VAL:HA	1:H:31:PHE:O	2.14	0.48
1:H:276:ILE:HA	1:H:280:MET:SD	2.53	0.48
1:A:138:SER:C	1:A:140:GLN:H	2.16	0.48
1:D:85:ASP:OD2	1:D:88:ALA:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:MET:CE	1:D:341:ASN:O	2.61	0.48
1:D:239:MET:H	1:D:244:ARG:HH11	1.59	0.48
1:D:343:LEU:HD23	1:D:347:VAL:CG2	2.43	0.48
1:H:10:ARG:HH11	1:H:76:ARG:HE	1.62	0.48
2:I:316:TYR:CD1	2:I:351:ARG:HG2	2.49	0.48
2:I:435:VAL:HG22	2:I:436:GLU:O	2.14	0.48
2:I:437:ASN:C	2:I:439:LEU:H	2.17	0.48
1:B:85:ASP:OD1	1:B:88:ALA:HB3	2.13	0.48
1:B:90:ILE:O	1:B:91:LYS:C	2.50	0.48
1:B:267:ILE:HD11	4:B:400:NAD:N1A	2.29	0.48
2:C:308:SER:HB2	2:C:384:ASP:OD2	2.14	0.48
2:C:425:LYS:HZ3	2:C:425:LYS:CB	2.27	0.48
1:D:223:ASP:HA	1:D:227:LYS:HG2	1.95	0.48
1:D:239:MET:HB2	1:D:244:ARG:NE	2.19	0.48
1:G:96:LEU:HB3	1:G:119:ALA:HB2	1.95	0.48
1:G:332:SER:HB2	1:G:333:PRO:HD3	1.95	0.48
2:I:439:LEU:O	2:I:441:PHE:N	2.47	0.48
2:C:420:THR:HB	1:H:162:MET:HE3	1.96	0.48
1:D:247:GLN:O	1:D:249:GLU:N	2.46	0.48
1:G:342:PHE:CE1	1:G:362:THR:HG23	2.48	0.48
1:H:13:GLU:HG2	1:H:74:VAL:HG21	1.96	0.48
1:H:98:CYS:O	1:H:121:ALA:HA	2.13	0.48
1:H:121:ALA:HB1	1:H:123:GLU:CD	2.32	0.48
1:H:245:LYS:C	1:H:247:GLN:H	2.16	0.48
1:H:367:CYS:SG	1:H:370:ARG:HD2	2.52	0.48
1:H:368:VAL:HG13	1:H:376:HIS:CB	2.43	0.48
1:A:120:TYR:HB3	1:A:366:THR:HG23	1.96	0.48
1:A:140:GLN:C	1:A:142:ASN:N	2.67	0.48
1:D:7:LYS:HB2	1:D:39:ALA:CB	2.43	0.48
1:D:36:GLU:HB3	1:D:39:ALA:HB2	1.96	0.48
1:D:68:ALA:H	1:D:91:LYS:CD	2.27	0.48
1:D:158:ARG:HG3	1:E:329:ALA:CB	2.43	0.48
1:D:340:LEU:C	1:D:340:LEU:HD23	2.33	0.48
1:A:138:SER:OG	4:A:400:NAD:H5N	2.12	0.48
1:B:93:GLY:HA2	1:B:116:LYS:O	2.14	0.48
2:C:371:PHE:HB2	2:C:376:ILE:CG1	2.43	0.48
1:E:135:ASP:O	1:E:137:LEU:N	2.47	0.48
1:E:156:PHE:CE2	1:E:158:ARG:HB2	2.49	0.48
2:F:377:ASN:OD1	2:F:413:LEU:HA	2.13	0.48
1:G:354:LEU:HD23	1:G:354:LEU:C	2.34	0.48
1:H:3:ILE:HG23	1:H:33:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:ARG:CG	1:H:327:VAL:HG22	2.44	0.48
1:A:180:VAL:O	1:A:180:VAL:HG12	2.14	0.48
1:B:50:LEU:O	1:B:53:ALA:N	2.46	0.48
1:B:207:THR:HA	1:B:210:GLN:HG3	1.96	0.48
1:D:343:LEU:O	1:D:347:VAL:HG23	2.14	0.48
1:E:37:GLN:HG2	1:E:59:SER:HA	1.95	0.48
1:E:78:MET:HA	1:E:82:GLU:OE2	2.14	0.48
1:E:161:PRO:HB3	1:E:195:GLY:HA3	1.96	0.48
1:G:97:MET:CE	1:G:343:LEU:HD13	2.43	0.48
1:H:203:VAL:HG13	4:H:400:NAD:N7A	2.28	0.48
1:H:361:GLU:HA	1:H:364:SER:OG	2.13	0.48
1:B:13:GLU:OE1	1:B:75:GLN:NE2	2.37	0.48
1:D:354:LEU:O	1:D:355:VAL:HG22	2.14	0.48
1:E:3:ILE:HA	1:E:70:VAL:O	2.14	0.48
1:H:91:LYS:O	1:H:94:ALA:HB2	2.14	0.48
1:A:7:LYS:H	1:A:36:GLU:CG	2.27	0.47
1:A:21:GLU:CD	1:A:21:GLU:N	2.68	0.47
1:B:265:ALA:CB	1:B:275:LEU:HD11	2.43	0.47
1:B:295:VAL:HG13	1:B:296:GLU:N	2.28	0.47
2:C:444:ASN:C	2:C:444:ASN:HD22	2.17	0.47
1:D:46:THR:O	1:D:49:ALA:N	2.46	0.47
1:D:57:ILE:HD12	1:D:58:ALA:O	2.14	0.47
1:D:125:MET:CE	1:D:134:MET:HB2	2.44	0.47
1:D:126:PRO:O	1:D:128:ILE:N	2.43	0.47
1:D:275:LEU:O	1:D:280:MET:HE1	2.14	0.47
1:E:120:TYR:HB3	1:E:366:THR:HG22	1.96	0.47
1:G:332:SER:O	1:G:333:PRO:C	2.53	0.47
1:H:98:CYS:H	1:H:122:MET:HE1	1.79	0.47
1:B:1:MET:HE1	1:B:353:THR:HA	1.96	0.47
1:B:113:THR:CG2	1:B:373:ALA:HA	2.40	0.47
1:E:302:PRO:HG2	1:E:303:LEU:HD12	1.97	0.47
1:H:47:ASP:HB3	1:H:57:ILE:CG1	2.43	0.47
1:H:330:ASP:O	1:H:333:PRO:HD2	2.14	0.47
2:C:425:LYS:HZ3	2:C:425:LYS:HB3	1.78	0.47
1:D:47:ASP:OD2	1:D:57:ILE:HD13	2.14	0.47
1:D:202:ASP:HB3	1:D:207:THR:HG21	1.96	0.47
1:E:123:GLU:HA	1:E:137:LEU:HD11	1.95	0.47
1:E:220:THR:O	1:E:221:VAL:C	2.52	0.47
1:A:158:ARG:HG3	1:B:329:ALA:HB3	1.95	0.47
1:A:177:VAL:O	1:A:177:VAL:HG13	2.14	0.47
1:B:325:SER:O	1:B:328:ALA:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ASN:HD22	1:D:325:SER:CB	2.16	0.47
1:D:354:LEU:C	1:D:355:VAL:CG2	2.83	0.47
2:F:393:ASP:O	2:F:395:THR:N	2.47	0.47
2:I:295:GLY:HA3	2:I:446:MET:CE	2.44	0.47
1:A:5:ILE:HG21	1:A:18:ILE:HG22	1.97	0.47
1:B:72:TRP:CD2	1:B:339:LEU:HD23	2.49	0.47
1:B:96:LEU:HD12	1:B:97:MET:N	2.29	0.47
1:B:120:TYR:HE1	1:B:367:CYS:HB2	1.79	0.47
1:D:199:MET:HG2	1:D:219:ILE:HD11	1.97	0.47
1:E:46:THR:O	1:E:50:LEU:HB2	2.13	0.47
1:E:155:GLU:HG3	1:E:318:VAL:HG21	1.96	0.47
2:F:405:SER:C	2:F:407:ILE:H	2.18	0.47
1:G:5:ILE:HG23	1:G:17:ALA:HB3	1.96	0.47
1:G:174:ARG:HB2	1:G:258:THR:HA	1.97	0.47
1:H:3:ILE:CG1	1:H:70:VAL:HG13	2.45	0.47
1:H:128:ILE:O	1:H:132:GLN:HG2	2.14	0.47
1:H:129:SER:HA	1:H:132:GLN:NE2	2.29	0.47
2:I:363:ALA:O	2:I:364:ASN:HB2	2.14	0.47
1:B:105:ASN:HB3	1:B:108:VAL:HG12	1.97	0.47
2:C:330:MET:HB2	2:C:460:VAL:HG22	1.97	0.47
1:D:130:ARG:NH1	1:D:360:ASP:OD2	2.48	0.47
1:E:72:TRP:HE1	1:E:97:MET:HE2	1.79	0.47
1:E:210:GLN:H	1:E:210:GLN:HG2	1.37	0.47
2:F:334:LEU:HB3	2:F:339:VAL:HB	1.96	0.47
1:G:188:ILE:CG2	1:G:214:LEU:HD13	2.44	0.47
1:G:248:ALA:HB1	1:G:280:MET:HE1	1.95	0.47
1:G:346:HIS:CE1	1:G:363:VAL:CG2	2.98	0.47
1:A:1:MET:CE	1:A:1:MET:HA	2.44	0.47
1:A:28:GLY:C	1:A:30:GLY:H	2.17	0.47
1:A:207:THR:O	1:A:210:GLN:HB2	2.15	0.47
1:A:266:LEU:O	1:A:267:ILE:HG13	2.15	0.47
1:B:312:LYS:HE2	1:B:313:HIS:NE2	2.30	0.47
2:C:416:GLU:HG3	2:C:442:ARG:HH12	1.79	0.47
1:D:221:VAL:CG2	1:D:247:GLN:HA	2.45	0.47
1:D:248:ALA:HB1	1:D:280:MET:SD	2.55	0.47
1:D:320:HIS:CD2	1:D:326:ARG:CZ	2.98	0.47
1:E:1:MET:HG2	1:E:352:LYS:O	2.13	0.47
1:E:244:ARG:CB	1:E:244:ARG:NH2	2.75	0.47
1:H:347:VAL:O	1:H:347:VAL:HG13	2.14	0.47
2:I:397:PRO:HB3	2:I:416:GLU:OE2	2.15	0.47
2:I:426:ARG:NH2	6:I:500:NDP:O3X	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:439:LEU:C	2:I:441:PHE:N	2.68	0.47
1:A:15:ARG:NH1	1:A:324:PRO:HB2	2.30	0.47
1:B:2:LYS:N	1:B:69:ASP:OD1	2.41	0.47
1:D:68:ALA:O	1:D:91:LYS:HG2	2.14	0.47
1:E:127:ARG:HH22	1:E:132:GLN:HG3	1.78	0.47
1:H:25:LYS:HG2	1:H:340:LEU:HD21	1.97	0.47
1:A:106:ARG:O	1:A:109:VAL:N	2.47	0.47
1:A:377:PRO:HA	1:A:381:GLY:HA3	1.96	0.47
1:E:65:LEU:O	1:E:67:GLN:N	2.48	0.47
1:E:362:THR:HG23	1:E:363:VAL:HG23	1.97	0.47
2:F:326:ALA:O	2:F:329:GLU:HB2	2.15	0.47
2:F:414:ASP:HB3	2:F:417:LYS:HG3	1.96	0.47
1:G:208:LYS:HZ2	1:G:220:THR:HG23	1.80	0.47
1:G:256:VAL:HG23	1:G:257:LYS:HG3	1.97	0.47
1:H:112:LEU:CD1	1:H:112:LEU:H	2.28	0.47
2:I:416:GLU:OE1	2:I:442:ARG:NH1	2.48	0.47
2:I:433:ALA:O	2:I:435:VAL:N	2.47	0.47
1:B:267:ILE:HG12	4:B:400:NAD:C2A	2.45	0.47
2:C:343:TYR:N	2:C:343:TYR:CD1	2.83	0.47
1:D:94:ALA:O	1:D:117:ILE:HG23	2.15	0.47
1:D:358:LEU:CD1	1:D:370:ARG:HH22	2.18	0.47
1:E:169:THR:CG2	1:E:170:VAL:N	2.77	0.47
1:H:9:ARG:NH2	1:H:36:GLU:OE1	2.48	0.47
1:H:92:GLU:HB2	1:H:116:LYS:HZ3	1.78	0.47
1:B:8:GLU:OE1	1:B:74:VAL:HG22	2.15	0.46
1:E:23:VAL:HG11	1:E:55:ALA:HB2	1.97	0.46
1:E:136:ILE:HD12	1:E:137:LEU:N	2.30	0.46
2:F:403:PRO:HA	2:F:408:TYR:CD1	2.49	0.46
1:H:18:ILE:CD1	1:H:23:VAL:CG2	2.87	0.46
1:H:35:VAL:HG21	1:H:50:LEU:CD2	2.36	0.46
1:H:101:GLY:N	1:H:123:GLU:OE2	2.41	0.46
1:H:241:GLU:HG2	1:H:244:ARG:HB2	1.97	0.46
1:A:272:ALA:HB2	1:A:297:ALA:HB3	1.98	0.46
1:B:260:ILE:HD13	1:B:289:VAL:HG13	1.97	0.46
2:C:395:THR:OG1	2:C:415:VAL:HG21	2.15	0.46
2:C:423:PHE:C	2:C:424:ILE:HD12	2.35	0.46
1:D:351:THR:O	1:D:352:LYS:C	2.53	0.46
1:G:114:LYS:C	1:G:116:LYS:H	2.18	0.46
1:H:5:ILE:CG1	1:H:72:TRP:CD1	2.97	0.46
1:A:164:MET:CE	2:C:357:ASN:HD21	2.29	0.46
1:B:219:ILE:O	1:B:220:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:THR:HA	1:B:375:VAL:HG23	1.97	0.46
2:C:300:ALA:HB2	2:C:448:LEU:HD11	1.98	0.46
2:C:444:ASN:C	2:C:444:ASN:ND2	2.69	0.46
1:G:255:LEU:HD21	1:G:276:ILE:CD1	2.45	0.46
1:H:330:ASP:O	1:H:333:PRO:HG2	2.14	0.46
2:I:396:ASN:O	2:I:412:ILE:HD13	2.15	0.46
1:A:23:VAL:HG22	1:A:33:VAL:HG11	1.97	0.46
1:D:4:ALA:CB	1:D:34:ILE:HB	2.45	0.46
1:D:311:VAL:O	1:D:312:LYS:HG2	2.16	0.46
1:E:25:LYS:HG2	1:E:340:LEU:HD21	1.96	0.46
1:E:136:ILE:HD11	1:E:137:LEU:HD12	1.96	0.46
1:E:178:PHE:HB2	1:E:263:THR:HA	1.96	0.46
1:G:163:MET:HB2	1:G:170:VAL:HG13	1.94	0.46
1:B:5:ILE:O	1:B:35:VAL:HA	2.15	0.46
1:B:128:ILE:HD12	1:B:130:ARG:CD	2.32	0.46
1:B:366:THR:HG22	1:B:367:CYS:N	2.30	0.46
2:C:403:PRO:HG3	2:C:408:TYR:CZ	2.51	0.46
2:C:425:LYS:CB	2:C:425:LYS:NZ	2.79	0.46
1:D:280:MET:C	1:D:282:THR:N	2.69	0.46
1:E:17:ALA:O	1:E:18:ILE:HB	2.15	0.46
1:E:110:GLU:O	1:E:113:THR:HB	2.15	0.46
2:F:452:ALA:H	6:F:500:NDP:C2A	2.28	0.46
2:I:453:LYS:HE2	2:I:457:GLU:OE2	2.16	0.46
1:B:50:LEU:HB3	1:B:55:ALA:HB3	1.97	0.46
2:C:322:GLN:HE22	2:C:324:GLN:HE22	1.60	0.46
1:D:19:SER:OG	1:D:22:VAL:HG23	2.15	0.46
1:D:318:VAL:HG13	1:D:320:HIS:CE1	2.51	0.46
1:E:341:ASN:O	1:E:345:PRO:CD	2.63	0.46
1:G:373:ALA:O	1:G:375:VAL:HG13	2.16	0.46
1:H:264:THR:O	1:H:265:ALA:C	2.53	0.46
1:H:281:VAL:HG21	1:H:303:LEU:HD11	1.98	0.46
1:H:354:LEU:H	1:H:354:LEU:CD2	2.09	0.46
1:A:165:THR:CG2	2:C:353:PRO:HB3	2.42	0.46
1:A:351:THR:HB	1:A:353:THR:HG22	1.98	0.46
1:B:207:THR:O	1:B:210:GLN:N	2.49	0.46
2:C:317:GLY:HA3	2:C:390:GLY:CA	2.46	0.46
1:D:16:VAL:HG22	1:D:18:ILE:HG22	1.97	0.46
1:D:91:LYS:C	1:D:92:GLU:O	2.52	0.46
1:E:344:THR:N	1:E:345:PRO:CD	2.79	0.46
2:F:328:ARG:HB3	2:F:328:ARG:CZ	2.45	0.46
1:H:5:ILE:HD11	1:H:72:TRP:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:VAL:O	1:B:112:LEU:CD1	2.61	0.46
1:B:188:ILE:HD11	1:B:200:ALA:HB2	1.98	0.46
1:D:113:THR:CA	1:D:369:THR:HG21	2.46	0.46
1:D:146:TYR:CE2	1:E:159:ALA:HA	2.51	0.46
1:D:344:THR:N	1:D:345:PRO:CD	2.78	0.46
1:G:47:ASP:HB3	1:G:57:ILE:HG12	1.98	0.46
1:H:40:GLY:O	1:H:43:ALA:N	2.47	0.46
1:H:295:VAL:HG11	1:H:319:GLY:CA	2.46	0.46
1:H:348:ASP:N	1:H:355:VAL:HG12	2.31	0.46
1:A:120:TYR:HD2	1:A:366:THR:HG22	1.81	0.46
2:C:330:MET:HG3	2:C:463:MET:CE	2.42	0.46
1:D:120:TYR:CE1	1:D:363:VAL:HG13	2.50	0.46
1:E:112:LEU:HB3	1:E:117:ILE:HB	1.98	0.46
1:E:136:ILE:HG22	1:E:338:ASN:CB	2.45	0.46
1:H:3:ILE:HG13	1:H:70:VAL:HG13	1.97	0.46
1:H:218:PHE:HD2	1:H:220:THR:CG2	2.25	0.46
2:I:399:ALA:CA	2:I:408:TYR:HA	2.34	0.46
1:D:13:GLU:OE1	1:D:13:GLU:HA	2.16	0.46
1:D:113:THR:HA	1:D:369:THR:CG2	2.44	0.46
1:D:360:ASP:C	1:D:362:THR:H	2.18	0.46
1:E:19:SER:OG	1:E:22:VAL:HG23	2.16	0.46
1:E:327:VAL:O	1:E:327:VAL:HG12	2.16	0.46
2:F:453:LYS:HE2	2:F:457:GLU:OE2	2.16	0.46
1:H:210:GLN:HA	1:H:213:SER:HB3	1.97	0.46
1:A:38:GLY:N	1:A:47:ASP:OD1	2.48	0.45
1:B:10:ARG:HH11	1:B:10:ARG:CG	2.29	0.45
1:B:10:ARG:NH1	1:B:76:ARG:O	2.49	0.45
1:B:190:THR:HA	1:B:193:ARG:HG2	1.98	0.45
1:B:346:HIS:HD1	1:B:356:MET:CE	2.29	0.45
2:C:416:GLU:HB3	2:C:439:LEU:HD21	1.98	0.45
1:E:25:LYS:CG	1:E:340:LEU:HD21	2.45	0.45
1:E:162:MET:HE1	2:I:420:THR:HG23	1.99	0.45
1:H:7:LYS:HB2	1:H:39:ALA:HB2	1.96	0.45
1:H:192:LYS:HE2	1:H:215:GLY:HA3	1.98	0.45
2:I:313:VAL:HG22	2:I:344:ALA:HB3	1.98	0.45
2:I:317:GLY:HA3	2:I:390:GLY:CA	2.46	0.45
1:B:295:VAL:HG11	1:B:320:HIS:O	2.16	0.45
2:C:366:PRO:HB2	2:C:369:GLU:HG3	1.98	0.45
1:D:198:VAL:HG12	1:D:199:MET:N	2.32	0.45
1:E:97:MET:O	1:E:98:CYS:CB	2.61	0.45
1:E:130:ARG:O	1:E:130:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ARG:O	1:E:148:ALA:C	2.55	0.45
1:E:368:VAL:O	1:E:368:VAL:HG12	2.16	0.45
1:H:41:VAL:HG13	1:H:42:GLY:N	2.32	0.45
1:H:131:ALA:HA	1:H:134:MET:HE3	1.97	0.45
1:H:204:ARG:C	1:H:206:ALA:H	2.20	0.45
2:I:455:MET:O	2:I:459:ILE:HG13	2.16	0.45
1:B:185:LEU:HD13	2:C:352:MET:HB3	1.97	0.45
2:C:330:MET:HG2	2:C:334:LEU:HD21	1.98	0.45
1:D:85:ASP:OD2	1:D:88:ALA:CB	2.63	0.45
1:D:255:LEU:C	1:D:257:LYS:H	2.19	0.45
2:F:437:ASN:C	2:F:439:LEU:N	2.68	0.45
1:G:266:LEU:H	4:G:400:NAD:H51A	1.81	0.45
1:H:100:LEU:CB	1:H:121:ALA:HB2	2.42	0.45
1:H:181:GLY:HA2	4:H:400:NAD:H52N	1.98	0.45
1:H:208:LYS:HZ2	1:H:220:THR:CG2	2.29	0.45
1:A:188:ILE:HG23	1:A:198:VAL:HG11	1.98	0.45
1:B:73:LYS:NZ	1:B:73:LYS:HB3	2.32	0.45
2:C:459:ILE:O	2:C:463:MET:HG3	2.16	0.45
1:D:22:VAL:HG21	1:D:336:ALA:HB1	1.97	0.45
1:D:29:LEU:CD2	1:D:347:VAL:HG11	2.46	0.45
1:E:130:ARG:HD3	2:F:409:GLY:HA3	1.99	0.45
2:F:318:MET:CE	2:F:324:GLN:HG2	2.47	0.45
1:G:265:ALA:HB2	1:G:275:LEU:HD11	1.99	0.45
1:H:65:LEU:O	1:H:66:SER:C	2.53	0.45
2:I:437:ASN:OD1	2:I:439:LEU:HB2	2.16	0.45
1:A:16:VAL:HG22	1:A:18:ILE:HG22	1.97	0.45
1:B:62:ALA:C	1:B:64:ALA:H	2.19	0.45
1:B:354:LEU:C	1:B:354:LEU:HD23	2.36	0.45
2:C:379:SER:O	2:C:380:PHE:C	2.54	0.45
1:D:16:VAL:O	1:D:16:VAL:HG13	2.17	0.45
1:E:207:THR:O	1:E:211:VAL:HG23	2.17	0.45
1:G:34:ILE:HG22	1:G:64:ALA:HB1	1.97	0.45
1:H:244:ARG:NH2	1:H:275:LEU:HD21	2.32	0.45
1:A:106:ARG:N	1:A:107:PRO:CD	2.75	0.45
2:C:362:GLU:O	2:C:362:GLU:HG2	2.15	0.45
1:D:97:MET:CE	1:D:343:LEU:HD12	2.47	0.45
1:D:240:GLY:O	1:D:242:GLU:N	2.49	0.45
1:E:342:PHE:CD1	1:E:342:PHE:C	2.89	0.45
2:F:376:ILE:O	2:F:376:ILE:HG12	2.15	0.45
2:F:401:THR:OG1	2:F:402:ASP:N	2.48	0.45
1:G:16:VAL:HG22	1:G:17:ALA:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:LYS:O	1:H:29:LEU:HD13	2.17	0.45
1:H:62:ALA:O	1:H:66:SER:N	2.50	0.45
2:I:440:PHE:HD2	2:I:447:MET:CE	2.29	0.45
1:B:281:VAL:HG23	1:B:313:HIS:HD2	1.81	0.45
1:B:346:HIS:O	1:B:348:ASP:N	2.49	0.45
1:E:369:THR:O	1:E:369:THR:CG2	2.64	0.45
1:G:92:GLU:H	1:G:92:GLU:HG2	1.52	0.45
1:G:221:VAL:HG12	1:G:222:ASP:H	1.80	0.45
1:H:3:ILE:O	1:H:33:VAL:HA	2.15	0.45
2:I:332:ASP:O	2:I:333:VAL:C	2.54	0.45
1:B:79:THR:O	1:B:84:THR:O	2.35	0.45
2:C:418:ALA:O	2:C:419:GLY:C	2.55	0.45
1:D:164:MET:HE2	1:D:169:THR:HG23	1.99	0.45
1:D:252:LEU:HD11	1:D:283:LYS:HD3	1.99	0.45
1:E:267:ILE:HG12	1:E:273:PRO:HD3	1.98	0.45
2:F:300:ALA:O	2:F:304:MET:HE2	2.17	0.45
1:H:245:LYS:C	1:H:247:GLN:N	2.70	0.45
1:B:272:ALA:HB1	1:B:300:ASN:ND2	2.32	0.45
2:C:453:LYS:O	2:C:457:GLU:HG3	2.17	0.45
1:D:23:VAL:O	1:D:26:LEU:HB2	2.17	0.45
1:D:332:SER:CB	1:D:333:PRO:HD3	2.45	0.45
2:F:445:THR:CG2	2:F:446:MET:N	2.80	0.45
1:G:63:GLN:OE1	1:G:63:GLN:HA	2.16	0.45
1:A:3:ILE:HG13	1:A:70:VAL:HG13	1.99	0.45
1:B:87:VAL:C	1:B:89:LEU:H	2.20	0.45
1:B:276:ILE:O	1:B:301:CYS:HA	2.17	0.45
2:C:309:LYS:HE2	2:C:382:THR:O	2.17	0.45
1:D:160:PHE:CZ	1:D:260:ILE:HD12	2.51	0.45
1:G:270:LYS:HD2	1:G:270:LYS:N	2.31	0.45
1:H:63:GLN:HE21	1:H:63:GLN:CA	2.21	0.45
2:I:299:ASP:O	2:I:303:ILE:HG13	2.17	0.45
1:B:105:ASN:O	1:B:108:VAL:HG12	2.17	0.44
2:C:385:VAL:HG12	2:C:386:ALA:N	2.32	0.44
1:D:3:ILE:HB	1:D:70:VAL:CG2	2.47	0.44
1:D:57:ILE:HD12	1:D:58:ALA:N	2.30	0.44
1:D:65:LEU:HD22	1:D:71:VAL:HG13	1.99	0.44
1:E:272:ALA:HB3	1:E:299:GLY:H	1.82	0.44
1:G:101:GLY:N	1:G:123:GLU:OE2	2.50	0.44
1:H:66:SER:HB3	1:H:67:GLN:NE2	2.32	0.44
1:H:99:HIS:CE1	1:H:123:GLU:HB3	2.52	0.44
1:H:120:TYR:CB	1:H:366:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:325:SER:C	1:H:327:VAL:H	2.20	0.44
1:H:356:MET:O	1:H:358:LEU:N	2.50	0.44
1:A:18:ILE:N	1:A:336:ALA:HB2	2.32	0.44
1:B:244:ARG:HD3	1:B:244:ARG:N	2.28	0.44
2:C:420:THR:HG21	1:H:169:THR:OG1	2.18	0.44
1:E:143:LEU:HD13	1:E:327:VAL:HG11	2.00	0.44
1:E:284:MET:HE3	1:E:315:VAL:HG21	1.99	0.44
1:G:121:ALA:HB1	1:G:123:GLU:OE1	2.16	0.44
1:H:125:MET:HG3	1:H:131:ALA:HB1	1.97	0.44
1:A:167:ALA:HB2	1:B:338:ASN:ND2	2.31	0.44
1:B:147:ARG:HH11	1:B:151:ASP:CG	2.19	0.44
1:D:205:ALA:C	1:D:207:THR:N	2.71	0.44
1:D:277:THR:O	1:D:280:MET:N	2.46	0.44
1:D:362:THR:O	1:D:362:THR:CG2	2.65	0.44
1:E:132:GLN:O	1:E:133:SER:C	2.56	0.44
1:E:273:PRO:O	1:E:274:VAL:C	2.55	0.44
1:H:113:THR:HG21	1:H:374:ILE:CG1	2.43	0.44
2:I:396:ASN:HA	2:I:397:PRO:HD2	1.85	0.44
1:A:161:PRO:CB	1:B:193:ARG:HH12	2.29	0.44
1:A:277:THR:C	1:A:279:GLU:H	2.20	0.44
1:D:43:ALA:O	1:D:44:SER:HB2	2.18	0.44
1:D:149:VAL:HG11	1:D:190:THR:HG22	1.99	0.44
2:F:442:ARG:HG3	2:F:442:ARG:HH11	1.82	0.44
1:G:200:ALA:HB3	1:G:211:VAL:CG1	2.47	0.44
1:H:72:TRP:CA	1:H:97:MET:O	2.64	0.44
1:B:3:ILE:HG23	1:B:3:ILE:O	2.17	0.44
2:C:373:LEU:HD11	2:C:411:PRO:HB2	1.99	0.44
2:C:401:THR:O	2:C:408:TYR:CE2	2.71	0.44
1:E:7:LYS:HE3	1:E:8:GLU:O	2.18	0.44
1:E:160:PHE:CE1	1:E:260:ILE:HD12	2.52	0.44
2:F:305:LYS:NZ	2:F:337:GLU:HG3	2.33	0.44
2:F:347:PRO:HD3	2:F:373:LEU:HB2	1.98	0.44
1:G:121:ALA:HB3	1:G:124:LEU:CD1	2.45	0.44
1:H:75:GLN:O	1:H:76:ARG:C	2.55	0.44
1:A:161:PRO:HB3	1:B:193:ARG:NH1	2.32	0.44
2:C:373:LEU:HG	2:C:377:ASN:HD21	1.81	0.44
1:D:9:ARG:CB	1:D:9:ARG:HH11	2.31	0.44
1:D:294:ALA:O	1:D:299:GLY:HA2	2.17	0.44
1:D:334:LEU:HD22	1:E:167:ALA:HB1	1.99	0.44
1:E:338:ASN:HD22	1:E:338:ASN:HA	1.64	0.44
1:G:163:MET:HB2	1:G:170:VAL:HG12	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:SER:O	1:H:91:LYS:HB2	2.17	0.44
1:A:105:ASN:C	1:A:107:PRO:HD2	2.38	0.44
1:A:118:THR:HA	1:A:369:THR:O	2.18	0.44
1:A:176:LEU:HD13	1:A:178:PHE:CZ	2.53	0.44
1:A:359:GLU:CD	1:A:359:GLU:H	2.21	0.44
1:D:362:THR:O	1:D:362:THR:HG23	2.17	0.44
1:E:122:MET:HE2	1:E:339:LEU:HG	1.99	0.44
1:G:10:ARG:CG	1:G:75:GLN:HG2	2.46	0.44
1:G:16:VAL:HG22	1:G:17:ALA:N	2.33	0.44
1:G:165:THR:CG2	2:I:353:PRO:HB3	2.47	0.44
1:G:247:GLN:C	1:G:249:GLU:H	2.21	0.44
1:G:278:GLU:HG3	1:G:303:LEU:CD1	2.48	0.44
1:H:119:ALA:H	1:H:369:THR:HG23	1.83	0.44
1:H:122:MET:N	1:H:122:MET:SD	2.91	0.44
1:A:337:LYS:HZ2	1:B:168:GLY:HA3	1.82	0.44
1:B:71:VAL:CG1	1:B:96:LEU:HD13	2.48	0.44
2:C:292:HIS:O	2:C:292:HIS:CD2	2.71	0.44
1:E:51:THR:CG2	1:E:57:ILE:HG23	2.48	0.44
1:G:184:GLY:O	1:G:188:ILE:HG13	2.17	0.44
1:H:33:VAL:HB	1:H:55:ALA:HB2	1.99	0.44
1:H:284:MET:CE	1:H:290:ILE:HD11	2.48	0.44
1:B:121:ALA:HB3	1:B:124:LEU:HD12	1.98	0.44
2:C:438:GLU:O	2:C:438:GLU:HG2	2.17	0.44
1:D:203:VAL:O	1:D:228:THR:HB	2.17	0.44
1:G:37:GLN:HE21	1:G:59:SER:HA	1.82	0.44
1:H:10:ARG:HH22	1:H:82:GLU:CD	2.21	0.44
1:H:19:SER:HB3	1:H:22:VAL:HB	2.00	0.44
1:A:175:VAL:HG12	1:A:176:LEU:N	2.33	0.43
1:A:351:THR:O	1:A:352:LYS:C	2.56	0.43
1:A:354:LEU:HD21	1:A:356:MET:HE1	1.93	0.43
1:B:100:LEU:O	1:B:101:GLY:C	2.56	0.43
1:D:24:LYS:C	1:D:26:LEU:H	2.21	0.43
1:D:109:VAL:CG2	1:D:110:GLU:N	2.81	0.43
1:G:110:GLU:O	1:G:114:LYS:HG2	2.18	0.43
1:A:120:TYR:CZ	1:A:356:MET:HG2	2.53	0.43
1:A:139:SER:OG	1:A:338:ASN:ND2	2.42	0.43
1:B:129:SER:O	1:B:132:GLN:HG3	2.17	0.43
1:E:7:LYS:HB2	1:E:39:ALA:CA	2.48	0.43
1:E:100:LEU:HD12	1:E:121:ALA:HB2	2.00	0.43
1:E:117:ILE:O	1:E:369:THR:HG23	2.18	0.43
1:G:10:ARG:HG3	1:G:11:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:LYS:HZ2	1:G:218:PHE:HD2	1.66	0.43
1:G:214:LEU:HD23	1:G:214:LEU:HA	1.85	0.43
1:H:67:GLN:NE2	1:H:67:GLN:N	2.56	0.43
1:H:346:HIS:HB3	1:H:356:MET:HA	1.99	0.43
1:H:347:VAL:CA	1:H:355:VAL:HG12	2.47	0.43
1:H:368:VAL:HG22	1:H:376:HIS:HB2	2.00	0.43
2:C:330:MET:HB2	2:C:460:VAL:CG2	2.48	0.43
1:D:2:LYS:HZ3	1:D:32:GLU:HG2	1.83	0.43
1:D:194:LEU:CD2	1:E:194:LEU:HD13	2.47	0.43
1:D:241:GLU:O	1:D:241:GLU:OE2	2.36	0.43
1:E:247:GLN:O	1:E:251:VAL:HG23	2.18	0.43
1:E:346:HIS:HB3	1:E:356:MET:HA	1.99	0.43
2:F:298:GLU:CD	2:F:298:GLU:H	2.22	0.43
1:G:156:PHE:CZ	1:G:259:ASP:HB3	2.54	0.43
1:G:200:ALA:O	1:G:218:PHE:HA	2.19	0.43
1:G:329:ALA:HB3	1:H:157:ALA:O	2.18	0.43
1:A:357:LYS:O	1:A:359:GLU:OE2	2.36	0.43
2:C:326:ALA:HB1	2:C:456:THR:HB	2.01	0.43
2:C:405:SER:HA	2:C:406:PRO:HD3	1.73	0.43
1:D:348:ASP:OD2	1:D:353:THR:N	2.46	0.43
1:G:199:MET:HE3	1:G:217:LYS:HB2	2.00	0.43
1:G:244:ARG:O	1:G:244:ARG:CG	2.65	0.43
1:H:120:TYR:CB	1:H:366:THR:HG21	2.45	0.43
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.82	0.43
1:B:36:GLU:O	1:B:39:ALA:HB2	2.18	0.43
1:B:62:ALA:C	1:B:64:ALA:N	2.72	0.43
1:D:9:ARG:NH1	1:D:9:ARG:HB3	2.33	0.43
1:D:100:LEU:O	1:D:102:ALA:N	2.51	0.43
1:D:255:LEU:C	1:D:257:LYS:N	2.71	0.43
1:E:23:VAL:CG1	1:E:55:ALA:HB2	2.49	0.43
1:E:220:THR:HG23	1:E:221:VAL:N	2.34	0.43
1:H:73:LYS:CD	1:H:75:GLN:O	2.66	0.43
1:H:128:ILE:HD11	1:H:131:ALA:H	1.84	0.43
1:H:213:SER:OG	2:I:355:HIS:CE1	2.71	0.43
1:A:62:ALA:HA	1:A:89:LEU:HD22	2.00	0.43
1:B:85:ASP:OD1	1:B:88:ALA:CB	2.66	0.43
1:B:99:HIS:CD2	1:B:99:HIS:C	2.92	0.43
1:D:5:ILE:HD13	1:D:18:ILE:HG13	2.01	0.43
1:D:193:ARG:C	1:D:195:GLY:H	2.22	0.43
1:D:264:THR:CG2	1:D:293:LEU:HD12	2.44	0.43
1:E:190:THR:O	1:E:191:ALA:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:MET:O	1:E:283:LYS:N	2.45	0.43
1:E:370:ARG:O	1:E:371:ASP:C	2.57	0.43
1:G:26:LEU:O	1:G:29:LEU:HB2	2.18	0.43
1:G:207:THR:O	1:G:208:LYS:C	2.57	0.43
1:H:18:ILE:HG12	1:H:19:SER:H	1.83	0.43
1:H:66:SER:CB	1:H:67:GLN:NE2	2.81	0.43
1:B:2:LYS:HE3	1:B:32:GLU:OE1	2.18	0.43
1:B:134:MET:HE1	1:B:362:THR:HG21	2.00	0.43
2:C:377:ASN:OD1	2:C:413:LEU:HA	2.19	0.43
1:D:175:VAL:HG23	1:D:196:ALA:HB1	2.01	0.43
2:F:416:GLU:HG3	2:F:439:LEU:CD1	2.48	0.43
1:A:205:ALA:C	1:A:207:THR:N	2.72	0.43
1:D:211:VAL:HG12	1:D:216:GLY:O	2.19	0.43
1:D:356:MET:HB3	1:D:363:VAL:HG11	2.00	0.43
1:G:247:GLN:O	1:G:249:GLU:N	2.52	0.43
1:H:29:LEU:HD21	1:H:344:THR:HG22	2.01	0.43
1:H:113:THR:C	1:H:115:ARG:H	2.20	0.43
1:H:128:ILE:HD11	1:H:131:ALA:CB	2.48	0.43
1:H:185:LEU:O	1:H:214:LEU:CD1	2.67	0.43
1:H:282:THR:HG22	1:H:313:HIS:NE2	2.34	0.43
1:H:346:HIS:CB	1:H:356:MET:HA	2.48	0.43
1:A:291:ILE:CD1	1:A:318:VAL:HB	2.40	0.43
1:B:152:GLY:HA2	1:B:291:ILE:HD11	2.01	0.43
1:B:202:ASP:OD1	1:B:203:VAL:N	2.51	0.43
1:B:308:LYS:CG	1:B:309:ILE:H	2.26	0.43
1:B:357:LYS:O	1:B:360:ASP:HB3	2.19	0.43
1:D:78:MET:CE	1:D:82:GLU:HG2	2.49	0.43
1:D:147:ARG:HG2	1:D:323:VAL:HG13	2.01	0.43
1:D:175:VAL:HA	1:D:260:ILE:O	2.19	0.43
1:D:292:ASP:OD2	1:D:300:ASN:N	2.52	0.43
1:D:361:GLU:CA	1:D:364:SER:HB3	2.31	0.43
1:E:120:TYR:HA	1:E:367:CYS:HA	2.00	0.43
2:F:316:TYR:HB2	2:F:350:GLY:HA2	2.00	0.43
2:F:352:MET:N	6:F:500:NDP:N7N	2.66	0.43
2:F:437:ASN:O	2:F:439:LEU:N	2.52	0.43
2:F:460:VAL:O	2:F:460:VAL:HG12	2.19	0.43
1:H:202:ASP:O	1:H:218:PHE:HZ	2.01	0.43
1:H:278:GLU:OE1	1:H:312:LYS:HE2	2.19	0.43
1:B:210:GLN:HE22	2:C:351:ARG:HD2	1.84	0.43
1:G:95:VAL:HA	1:G:118:THR:O	2.18	0.43
1:H:285:LYS:HA	1:H:286:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:355:VAL:O	1:H:355:VAL:CG1	2.65	0.43
1:A:78:MET:HG3	1:A:86:GLU:OE1	2.19	0.42
1:A:245:LYS:HD2	1:A:245:LYS:HA	1.86	0.42
1:A:343:LEU:HD23	1:A:343:LEU:C	2.39	0.42
1:B:87:VAL:HG13	1:B:88:ALA:H	1.81	0.42
1:B:130:ARG:H	1:B:130:ARG:HG3	1.44	0.42
1:E:4:ALA:HA	1:E:34:ILE:O	2.19	0.42
2:F:430:SER:OG	2:F:434:GLY:HA2	2.19	0.42
1:H:65:LEU:HB3	1:H:90:ILE:HA	2.01	0.42
1:D:121:ALA:HB1	1:D:124:LEU:HD22	2.01	0.42
1:E:65:LEU:HD12	1:E:89:LEU:HB2	2.01	0.42
2:F:442:ARG:HA	2:F:442:ARG:HD3	1.57	0.42
1:G:380:THR:O	1:G:380:THR:CG2	2.68	0.42
1:H:148:ALA:HB1	1:H:262:ILE:HG21	2.00	0.42
1:H:323:VAL:N	1:H:324:PRO:CD	2.82	0.42
1:A:136:ILE:HA	1:A:338:ASN:ND2	2.34	0.42
1:B:88:ALA:HA	1:B:115:ARG:HD2	2.01	0.42
1:D:68:ALA:N	1:D:91:LYS:CD	2.83	0.42
1:D:127:ARG:NE	1:D:235:TYR:CE2	2.87	0.42
1:D:163:MET:HB2	1:D:163:MET:HE2	1.84	0.42
1:E:97:MET:HE2	1:E:343:LEU:HD12	2.00	0.42
1:E:309:ILE:HG23	1:E:318:VAL:HG22	2.00	0.42
2:F:292:HIS:O	2:F:293:MET:CB	2.68	0.42
1:G:97:MET:O	1:G:98:CYS:HB3	2.18	0.42
1:H:72:TRP:CB	1:H:97:MET:HB2	2.25	0.42
1:A:343:LEU:HD23	1:A:343:LEU:O	2.19	0.42
2:C:317:GLY:HA3	2:C:390:GLY:HA3	2.02	0.42
2:C:365:VAL:HA	2:C:366:PRO:HD3	1.75	0.42
1:D:18:ILE:CD1	1:D:50:LEU:HD23	2.50	0.42
1:D:26:LEU:HD23	1:D:26:LEU:HA	1.89	0.42
1:E:23:VAL:HG21	1:E:50:LEU:CD1	2.49	0.42
1:H:71:VAL:O	1:H:96:LEU:HA	2.20	0.42
1:A:73:LYS:HB3	1:A:73:LYS:HE3	1.76	0.42
1:A:118:THR:HA	1:A:370:ARG:HA	2.01	0.42
1:B:348:ASP:CG	1:B:351:THR:HB	2.40	0.42
1:D:231:THR:O	1:D:232:ALA:C	2.58	0.42
1:D:263:THR:HB	1:D:300:ASN:HB2	2.02	0.42
1:D:343:LEU:HD23	1:D:347:VAL:HG22	2.02	0.42
1:E:112:LEU:HD12	1:E:112:LEU:N	2.32	0.42
1:E:362:THR:CG2	1:E:363:VAL:HG23	2.50	0.42
2:F:296:SER:OG	2:F:298:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:THR:HB	1:G:370:ARG:HA	2.02	0.42
1:G:172:PRO:HB3	2:I:367:TYR:HE2	1.84	0.42
1:G:243:PHE:C	1:G:245:LYS:N	2.64	0.42
2:I:380:PHE:O	2:I:383:ALA:HB3	2.20	0.42
1:A:5:ILE:O	1:A:35:VAL:HA	2.19	0.42
1:B:78:MET:N	1:B:86:GLU:OE1	2.47	0.42
1:B:197:VAL:O	1:B:197:VAL:HG12	2.19	0.42
1:B:303:LEU:HB2	1:B:317:ILE:HD13	2.01	0.42
1:D:120:TYR:CZ	1:D:356:MET:HG2	2.54	0.42
1:E:106:ARG:N	1:E:107:PRO:CD	2.82	0.42
1:E:268:PRO:O	1:E:270:LYS:N	2.53	0.42
2:I:454:LYS:HG3	2:I:455:MET:N	2.35	0.42
1:D:247:GLN:C	1:D:249:GLU:H	2.23	0.42
1:E:121:ALA:C	1:E:366:THR:HG23	2.40	0.42
1:G:76:ARG:HD3	1:G:100:LEU:O	2.19	0.42
1:G:295:VAL:HG21	1:G:306:PRO:HA	2.01	0.42
1:A:177:VAL:HA	1:A:262:ILE:O	2.19	0.42
1:A:290:ILE:HD12	1:A:317:ILE:CD1	2.49	0.42
1:A:327:VAL:O	1:A:328:ALA:C	2.58	0.42
1:A:362:THR:HG22	1:A:363:VAL:HG23	2.01	0.42
1:B:281:VAL:HG23	1:B:313:HIS:CD2	2.54	0.42
1:D:72:TRP:CE2	1:D:339:LEU:HB3	2.54	0.42
1:D:204:ARG:O	1:D:206:ALA:N	2.53	0.42
1:D:320:HIS:CD2	1:D:326:ARG:NH2	2.88	0.42
1:G:128:ILE:C	1:G:130:ARG:H	2.23	0.42
1:H:370:ARG:O	1:H:371:ASP:C	2.57	0.42
2:I:393:ASP:OD2	6:I:500:NDP:O3D	2.35	0.42
1:A:302:PRO:HG2	1:A:303:LEU:HD12	2.02	0.42
1:B:58:ALA:HB3	1:B:64:ALA:HB2	2.01	0.42
1:B:187:ALA:O	1:B:188:ILE:C	2.57	0.42
2:C:399:ALA:HB2	2:C:407:ILE:CD1	2.49	0.42
1:D:51:THR:OG1	1:D:57:ILE:HG22	2.20	0.42
1:E:138:SER:O	1:E:139:SER:C	2.58	0.42
2:F:292:HIS:O	2:F:293:MET:HB2	2.20	0.42
1:G:379:LEU:HD22	1:G:379:LEU:N	2.35	0.42
1:H:22:VAL:HG21	1:H:336:ALA:HB1	2.02	0.42
1:H:281:VAL:CG2	1:H:282:THR:N	2.83	0.42
2:I:318:MET:O	2:I:322:GLN:N	2.52	0.42
2:I:405:SER:OG	2:I:406:PRO:HD2	2.20	0.42
1:A:3:ILE:HD13	1:A:26:LEU:HD13	2.02	0.42
1:A:264:THR:CG2	1:A:293:LEU:HD12	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:HD22	1:A:323:VAL:HG21	2.01	0.42
1:B:67:GLN:OE1	1:B:67:GLN:N	2.44	0.42
1:B:80:ALA:HB2	1:B:85:ASP:OD2	2.20	0.42
2:C:394:VAL:HG22	6:C:500:NDP:O1N	2.20	0.42
2:C:415:VAL:C	2:C:417:LYS:H	2.23	0.42
1:D:356:MET:SD	1:D:356:MET:N	2.93	0.42
1:E:143:LEU:HD13	1:E:327:VAL:CG1	2.50	0.42
1:E:325:SER:C	1:E:327:VAL:H	2.23	0.42
2:F:429:ALA:HB3	6:F:500:NDP:O1X	2.18	0.42
2:F:439:LEU:C	2:F:441:PHE:H	2.24	0.42
1:H:46:THR:OG1	1:H:49:ALA:CB	2.68	0.42
1:A:179:GLY:O	1:A:184:GLY:HA3	2.20	0.41
1:A:368:VAL:O	1:A:368:VAL:HG12	2.20	0.41
1:B:352:LYS:HG2	1:B:352:LYS:O	2.20	0.41
2:C:416:GLU:HB3	2:C:439:LEU:CD2	2.50	0.41
1:D:17:ALA:O	1:D:18:ILE:HB	2.19	0.41
1:E:60:THR:HG22	1:E:63:GLN:CB	2.50	0.41
1:G:375:VAL:O	1:G:375:VAL:HG23	2.20	0.41
1:H:340:LEU:CD1	1:H:344:THR:CG2	2.98	0.41
1:A:115:ARG:HB2	1:A:117:ILE:HG12	2.01	0.41
1:A:207:THR:CG2	1:A:218:PHE:HE1	2.29	0.41
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.35	0.41
1:A:342:PHE:CD2	1:A:342:PHE:C	2.93	0.41
1:B:58:ALA:CB	1:B:64:ALA:HA	2.51	0.41
2:C:426:ARG:O	2:C:449:PHE:HD1	2.02	0.41
1:D:294:ALA:C	1:D:299:GLY:HA2	2.40	0.41
1:D:344:THR:CA	1:D:347:VAL:HG23	2.50	0.41
1:D:346:HIS:HD2	1:D:357:LYS:H	1.67	0.41
1:E:95:VAL:CG1	1:E:118:THR:HB	2.39	0.41
1:H:208:LYS:O	1:H:212:GLU:HB2	2.20	0.41
1:A:330:ASP:O	1:A:333:PRO:HD2	2.19	0.41
1:D:156:PHE:CZ	1:D:259:ASP:HB3	2.55	0.41
1:D:356:MET:HB3	1:D:363:VAL:HG21	2.02	0.41
1:E:3:ILE:CG2	1:E:33:VAL:HG22	2.50	0.41
2:F:365:VAL:O	2:F:366:PRO:C	2.59	0.41
1:G:20:PRO:HD3	1:G:45:ILE:HD13	2.03	0.41
1:H:143:LEU:HD23	1:H:143:LEU:HA	1.81	0.41
1:H:362:THR:HG23	1:H:363:VAL:HG23	2.02	0.41
1:A:118:THR:HG23	1:A:370:ARG:HB3	2.03	0.41
1:B:36:GLU:O	1:B:37:GLN:C	2.58	0.41
1:B:106:ARG:HH12	1:B:374:ILE:CD1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:VAL:O	1:E:16:VAL:HG13	2.20	0.41
1:G:153:ALA:HA	1:G:160:PHE:HE1	1.82	0.41
1:G:176:LEU:HD13	1:G:178:PHE:HE2	1.86	0.41
1:G:265:ALA:HA	4:G:400:NAD:O4B	2.19	0.41
1:G:361:GLU:H	1:G:361:GLU:HG2	1.48	0.41
1:H:241:GLU:CG	1:H:244:ARG:HB2	2.49	0.41
1:A:97:MET:O	1:A:98:CYS:HB3	2.19	0.41
1:B:181:GLY:O	1:B:182:VAL:C	2.59	0.41
1:B:242:GLU:O	1:B:245:LYS:CB	2.67	0.41
1:D:100:LEU:C	1:D:102:ALA:N	2.74	0.41
1:D:164:MET:CE	1:D:169:THR:HG23	2.50	0.41
1:D:224:GLU:N	1:D:227:LYS:HG2	2.35	0.41
1:G:9:ARG:O	1:G:10:ARG:C	2.59	0.41
1:G:346:HIS:ND1	1:G:356:MET:CE	2.84	0.41
1:H:29:LEU:HD12	1:H:29:LEU:N	2.35	0.41
1:H:73:LYS:HG3	1:H:98:CYS:SG	2.61	0.41
1:H:249:GLU:C	1:H:251:VAL:H	2.23	0.41
1:H:368:VAL:HG12	1:H:374:ILE:HG23	2.03	0.41
2:I:402:ASP:OD1	2:I:405:SER:HB2	2.19	0.41
1:A:205:ALA:C	1:A:207:THR:H	2.24	0.41
1:D:204:ARG:C	1:D:206:ALA:N	2.73	0.41
1:D:222:ASP:O	1:D:227:LYS:HE3	2.21	0.41
1:E:212:GLU:C	1:E:214:LEU:H	2.23	0.41
1:E:289:VAL:HA	1:E:316:LYS:O	2.20	0.41
1:E:330:ASP:O	1:E:333:PRO:HD2	2.20	0.41
1:E:348:ASP:OD1	1:E:352:LYS:N	2.53	0.41
1:G:122:MET:HG3	1:G:339:LEU:HD21	2.02	0.41
1:H:348:ASP:HB3	1:H:353:THR:HG22	2.02	0.41
1:A:138:SER:OG	4:A:400:NAD:C5N	2.68	0.41
1:B:10:ARG:HH12	1:B:76:ARG:HG2	1.85	0.41
1:B:73:LYS:CB	1:B:73:LYS:HZ2	2.33	0.41
1:B:299:GLY:C	1:B:301:CYS:H	2.23	0.41
2:C:331:ALA:O	2:C:335:LYS:HG3	2.20	0.41
1:D:122:MET:C	1:D:124:LEU:N	2.74	0.41
1:E:353:THR:HG22	1:E:354:LEU:O	2.20	0.41
2:F:454:LYS:CG	2:F:455:MET:N	2.83	0.41
1:G:3:ILE:HG13	1:G:70:VAL:HG13	2.03	0.41
1:G:346:HIS:HE1	1:G:363:VAL:CG2	2.34	0.41
1:H:180:VAL:HB	1:H:202:ASP:OD2	2.20	0.41
2:I:407:ILE:O	2:I:409:GLY:N	2.53	0.41
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG12	1:B:131:ALA:HB2	2.02	0.41
1:B:134:MET:HG2	1:B:342:PHE:CA	2.51	0.41
1:B:208:LYS:NZ	1:B:212:GLU:OE2	2.45	0.41
2:C:424:ILE:N	2:C:424:ILE:CD1	2.82	0.41
1:D:244:ARG:HD3	1:D:244:ARG:H	1.85	0.41
1:D:349:LYS:HD2	1:D:349:LYS:N	2.35	0.41
1:E:284:MET:HE1	1:E:290:ILE:HD11	2.02	0.41
1:E:343:LEU:HD23	1:E:343:LEU:C	2.41	0.41
1:E:358:LEU:H	1:E:358:LEU:CD1	2.15	0.41
1:G:96:LEU:HB3	1:G:119:ALA:CB	2.51	0.41
1:G:249:GLU:HA	1:G:249:GLU:OE1	2.21	0.41
1:G:280:MET:C	1:G:282:THR:N	2.72	0.41
1:H:25:LYS:HE3	1:H:25:LYS:CA	2.51	0.41
1:H:277:THR:O	1:H:278:GLU:C	2.58	0.41
1:A:340:LEU:HD12	1:A:340:LEU:HA	1.77	0.41
2:C:328:ARG:HD2	2:C:328:ARG:C	2.40	0.41
2:C:414:ASP:HB3	2:C:417:LYS:HG3	2.02	0.41
1:D:35:VAL:HG21	1:D:50:LEU:CD2	2.49	0.41
1:D:62:ALA:O	1:D:66:SER:HB3	2.20	0.41
1:D:65:LEU:HD23	1:D:65:LEU:N	2.36	0.41
1:D:138:SER:HA	1:D:141:SER:HB3	2.03	0.41
1:D:175:VAL:CG1	1:D:176:LEU:H	2.24	0.41
1:E:7:LYS:HB2	1:E:39:ALA:HB2	2.01	0.41
1:E:103:LEU:O	1:E:104:THR:HG23	2.20	0.41
1:E:311:VAL:O	1:E:311:VAL:HG13	2.20	0.41
2:F:425:LYS:HB2	6:F:500:NDP:O2X	2.21	0.41
1:G:176:LEU:HG	1:G:199:MET:HB3	2.03	0.41
1:G:277:THR:C	1:G:279:GLU:N	2.74	0.41
1:H:15:ARG:CG	1:H:15:ARG:NH2	2.83	0.41
1:H:50:LEU:HD12	1:H:50:LEU:HA	1.93	0.41
1:H:317:ILE:HD12	1:H:317:ILE:N	2.36	0.41
2:I:425:LYS:HB3	2:I:425:LYS:HE2	1.75	0.41
1:A:45:ILE:HG22	1:A:50:LEU:CD2	2.49	0.41
1:A:158:ARG:HB3	1:B:330:ASP:OD2	2.21	0.41
1:A:178:PHE:HB2	1:A:263:THR:HG22	2.01	0.41
1:B:155:GLU:HA	3:K:2:FRU:H61	2.02	0.41
2:C:399:ALA:CB	2:C:407:ILE:HG13	2.33	0.41
1:D:15:ARG:NH1	1:D:324:PRO:HB2	2.36	0.41
1:D:193:ARG:O	1:D:195:GLY:N	2.54	0.41
1:D:223:ASP:HB2	1:D:228:THR:OG1	2.21	0.41
1:D:305:GLU:HA	1:D:306:PRO:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:THR:HG23	1:E:84:THR:O	2.20	0.41
1:E:110:GLU:O	1:E:114:LYS:HG3	2.20	0.41
1:E:213:SER:O	2:F:322:GLN:NE2	2.54	0.41
2:F:321:ALA:O	2:F:322:GLN:HB2	2.21	0.41
1:G:128:ILE:HG13	1:G:130:ARG:H	1.86	0.41
1:H:2:LYS:O	1:H:70:VAL:HG12	2.21	0.41
1:H:61:ALA:O	1:H:65:LEU:HD13	2.20	0.41
1:H:143:LEU:HD12	1:H:331:ALA:HA	2.03	0.41
1:A:362:THR:CG2	1:A:363:VAL:N	2.83	0.40
1:B:5:ILE:CG2	1:B:17:ALA:HB3	2.51	0.40
1:B:267:ILE:HG12	4:B:400:NAD:N1A	2.36	0.40
2:C:425:LYS:NZ	6:C:500:NDP:O2B	2.54	0.40
2:C:454:LYS:HA	2:C:454:LYS:CE	2.43	0.40
1:D:125:MET:SD	1:D:126:PRO:HD2	2.61	0.40
1:E:72:TRP:CZ2	1:E:339:LEU:HB3	2.56	0.40
1:E:87:VAL:HG22	1:E:87:VAL:O	2.20	0.40
1:H:91:LYS:HE3	1:H:91:LYS:HB2	1.87	0.40
1:H:346:HIS:NE2	1:H:362:THR:CG2	2.83	0.40
1:B:24:LYS:H	1:B:24:LYS:HG3	1.68	0.40
1:B:158:ARG:HE	1:B:158:ARG:HB3	1.70	0.40
1:G:308:LYS:N	1:G:308:LYS:HD3	2.36	0.40
1:H:178:PHE:HD1	1:H:263:THR:HG22	1.87	0.40
1:A:28:GLY:C	1:A:30:GLY:N	2.74	0.40
1:A:122:MET:C	1:A:124:LEU:H	2.24	0.40
1:A:208:LYS:O	1:A:212:GLU:HG3	2.21	0.40
1:A:309:ILE:HG13	1:A:318:VAL:HG13	2.03	0.40
1:B:2:LYS:HB2	1:B:69:ASP:OD1	2.21	0.40
1:B:267:ILE:HD13	4:B:400:NAD:N1A	2.37	0.40
1:B:282:THR:HG22	1:B:313:HIS:CG	2.56	0.40
1:B:336:ALA:O	1:B:339:LEU:HB2	2.20	0.40
1:B:360:ASP:OD2	1:B:360:ASP:C	2.58	0.40
2:C:443:ASN:ND2	1:H:196:ALA:O	2.54	0.40
1:D:71:VAL:HB	1:D:96:LEU:HD12	2.03	0.40
1:D:100:LEU:O	1:D:101:GLY:C	2.60	0.40
2:F:345:ILE:CG1	2:F:370:VAL:HG13	2.51	0.40
2:F:432:TYR:CD2	6:F:500:NDP:H6N	2.55	0.40
1:G:47:ASP:O	1:G:51:THR:HG23	2.21	0.40
1:G:159:ALA:HA	1:H:146:TYR:CE2	2.55	0.40
1:H:51:THR:C	1:H:53:ALA:H	2.25	0.40
1:H:267:ILE:HA	1:H:268:PRO:HD2	1.86	0.40
1:H:349:LYS:H	1:H:349:LYS:HG2	1.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:301:ALA:O	2:I:305:LYS:HG2	2.21	0.40
2:I:318:MET:HB2	2:I:323:ALA:HB3	2.03	0.40
1:A:18:ILE:HD11	1:A:23:VAL:HG23	2.04	0.40
1:A:22:VAL:O	1:A:25:LYS:N	2.55	0.40
1:A:204:ARG:O	1:A:207:THR:HB	2.22	0.40
1:A:368:VAL:O	1:A:374:ILE:HG23	2.22	0.40
1:B:147:ARG:HD3	1:B:151:ASP:OD2	2.20	0.40
1:B:327:VAL:O	1:B:329:ALA:N	2.55	0.40
4:B:400:NAD:O1N	4:B:400:NAD:O3B	2.25	0.40
1:E:96:LEU:HD22	1:E:112:LEU:CD2	2.51	0.40
1:G:136:ILE:HG13	1:G:137:LEU:N	2.36	0.40
1:H:26:LEU:HD21	1:H:72:TRP:HZ2	1.85	0.40
1:H:147:ARG:HG3	1:H:327:VAL:CG2	2.50	0.40
2:I:318:MET:HE1	2:I:324:GLN:HB3	2.04	0.40
2:C:309:LYS:HE3	2:C:383:ALA:HB2	2.02	0.40
1:D:17:ALA:HB1	1:D:339:LEU:CD1	2.52	0.40
1:D:223:ASP:HA	1:D:227:LYS:CG	2.51	0.40
1:E:143:LEU:CD1	1:E:331:ALA:HB2	2.51	0.40
1:G:7:LYS:CG	1:G:39:ALA:HA	2.51	0.40
1:G:69:ASP:O	1:G:94:ALA:HB1	2.22	0.40
1:G:99:HIS:HB2	1:G:136:ILE:CD1	2.51	0.40
1:H:203:VAL:HG22	4:H:400:NAD:C8A	2.51	0.40
1:H:270:LYS:HB2	1:H:271:PRO:CD	2.51	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	359/384 (94%)	289 (80%)	51 (14%)	19 (5%)	2 12
1	B	355/384 (92%)	273 (77%)	57 (16%)	25 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	376/384 (98%)	277 (74%)	66 (18%)	33 (9%)	1 4
1	E	355/384 (92%)	265 (75%)	66 (19%)	24 (7%)	1 7
1	G	360/384 (94%)	292 (81%)	50 (14%)	18 (5%)	2 13
1	H	353/384 (92%)	258 (73%)	77 (22%)	18 (5%)	2 13
2	C	172/174 (99%)	133 (77%)	35 (20%)	4 (2%)	6 28
2	F	171/174 (98%)	141 (82%)	21 (12%)	9 (5%)	2 12
2	I	171/174 (98%)	125 (73%)	29 (17%)	17 (10%)	0 3
All	All	2672/2826 (95%)	2053 (77%)	452 (17%)	167 (6%)	1 8

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	LYS
1	A	357	LYS
1	A	358	LEU
1	A	378	ALA
1	B	371	ASP
1	D	18	ILE
1	D	66	SER
1	D	92	GLU
1	D	127	ARG
1	D	222	ASP
1	D	224	GLU
1	D	241	GLU
1	D	268	PRO
1	D	328	ALA
1	E	66	SER
1	E	98	CYS
1	E	328	ALA
1	E	348	ASP
1	E	356	MET
2	F	402	ASP
2	F	408	TYR
1	G	129	SER
1	G	248	ALA
1	G	274	VAL
1	G	357	LYS
2	I	324	GLN
2	I	378	SER
2	I	402	ASP

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Mol	Chain	Res	Type
2	I	463	MET
1	A	37	GLN
1	A	93	GLY
1	A	328	ALA
1	B	51	THR
1	B	66	SER
1	B	102	ALA
1	B	328	ALA
1	B	342	PHE
1	B	348	ASP
1	B	355	VAL
1	B	357	LYS
2	C	414	ASP
1	D	194	LEU
1	D	352	LYS
1	D	355	VAL
1	D	374	ILE
1	E	17	ALA
1	E	127	ARG
1	E	136	ILE
1	E	371	ASP
2	F	394	VAL
2	F	438	GLU
1	G	204	ARG
1	G	221	VAL
1	G	244	ARG
1	G	358	LEU
1	H	180	VAL
1	H	295	VAL
1	H	357	LYS
1	H	361	GLU
2	I	374	GLU
2	I	379	SER
2	I	408	TYR
1	A	82	GLU
1	A	127	ARG
1	A	278	GLU
1	A	304	SER
1	A	346	HIS
1	A	371	ASP
1	B	37	GLN
1	B	88	ALA

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Mol	Chain	Res	Type
1	B	127	ARG
1	B	157	ALA
1	B	268	PRO
1	B	340	LEU
1	B	378	ALA
2	C	373	LEU
2	C	380	PHE
2	C	416	GLU
1	D	64	ALA
1	D	102	ALA
1	D	232	ALA
1	D	357	LYS
1	E	87	VAL
1	E	104	THR
1	E	196	ALA
1	E	204	ARG
1	E	274	VAL
1	E	357	LYS
2	F	293	MET
1	G	92	GLU
1	G	111	ALA
1	G	348	ASP
1	G	371	ASP
1	H	66	SER
1	H	128	ILE
1	H	244	ARG
1	H	265	ALA
1	H	338	ASN
1	H	344	THR
1	H	354	LEU
2	I	414	ASP
2	I	431	GLY
2	I	434	GLY
2	I	438	GLU
2	I	440	PHE
1	A	114	LYS
1	B	116	LYS
1	B	158	ARG
1	B	187	ALA
1	B	188	ILE
1	B	349	LYS
1	D	74	VAL

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Mol	Chain	Res	Type
1	D	76	ARG
1	D	83	GLY
1	D	176	LEU
1	D	205	ALA
1	D	238	GLU
1	E	358	LEU
2	F	324	GLN
2	F	347	PRO
2	F	373	LEU
1	H	11	PRO
1	H	98	CYS
2	I	293	MET
2	I	452	ALA
1	A	103	LEU
1	B	6	PRO
1	D	98	CYS
1	D	141	SER
1	D	358	LEU
1	E	65	LEU
1	E	129	SER
1	G	322	ASN
1	G	369	THR
2	I	444	ASN
1	D	77	PRO
1	D	281	VAL
1	E	269	GLY
1	G	110	GLU
1	G	295	VAL
1	H	103	LEU
1	H	125	MET
1	H	205	ALA
1	H	358	LEU
2	I	316	TYR
2	I	339	VAL
1	A	305	GLU
1	D	20	PRO
1	E	355	VAL
1	H	355	VAL
1	B	128	ILE
1	D	306	PRO
1	G	375	VAL
1	G	377	PRO

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Mol	Chain	Res	Type
1	B	377	PRO
1	D	299	GLY
1	E	18	ILE
1	E	306	PRO
2	F	376	ILE
1	B	179	GLY
1	D	23	VAL
1	D	327	VAL
1	E	180	VAL
1	A	6	PRO
1	A	83	GLY
1	A	375	VAL
1	E	345	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	284/296 (96%)	254 (89%)	30 (11%)	6 26
1	B	281/296 (95%)	253 (90%)	28 (10%)	7 28
1	D	293/296 (99%)	255 (87%)	38 (13%)	4 18
1	E	281/296 (95%)	257 (92%)	24 (8%)	10 37
1	G	284/296 (96%)	260 (92%)	24 (8%)	10 37
1	H	280/296 (95%)	243 (87%)	37 (13%)	4 17
2	C	138/138 (100%)	125 (91%)	13 (9%)	8 32
2	F	137/138 (99%)	128 (93%)	9 (7%)	16 47
2	I	137/138 (99%)	128 (93%)	9 (7%)	16 47
All	All	2115/2190 (97%)	1903 (90%)	212 (10%)	7 28

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS

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Mol	Chain	Res	Type
1	A	41	VAL
1	A	46	THR
1	A	51	THR
1	A	76	ARG
1	A	81	GLU
1	A	84	THR
1	A	91	LYS
1	A	95	VAL
1	A	96	LEU
1	A	110	GLU
1	A	127	ARG
1	A	164	MET
1	A	170	VAL
1	A	176	LEU
1	A	199	MET
1	A	203	VAL
1	A	211	VAL
1	A	217	LYS
1	A	222	ASP
1	A	243	PHE
1	A	270	LYS
1	A	271	PRO
1	A	305	GLU
1	A	348	ASP
1	A	350	ASP
1	A	354	LEU
1	A	358	LEU
1	A	362	THR
1	A	366	THR
1	B	1	MET
1	B	19	SER
1	B	65	LEU
1	B	71	VAL
1	B	107	PRO
1	B	115	ARG
1	B	130	ARG
1	B	134	MET
1	B	147	ARG
1	B	164	MET
1	B	176	LEU
1	B	194	LEU
1	B	217	LYS

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Mol	Chain	Res	Type
1	B	244	ARG
1	B	252	LEU
1	B	267	ILE
1	B	277	THR
1	B	279	GLU
1	B	289	VAL
1	B	296	GLU
1	B	325	SER
1	B	344	THR
1	B	348	ASP
1	B	350	ASP
1	B	354	LEU
1	B	358	LEU
1	B	369	THR
1	B	371	ASP
2	C	291	ARG
2	C	298	GLU
2	C	318	MET
2	C	358	VAL
2	C	372	GLU
2	C	376	ILE
2	C	382	THR
2	C	416	GLU
2	C	420	THR
2	C	425	LYS
2	C	444	ASN
2	C	454	LYS
2	C	464	ASN
1	D	8	GLU
1	D	13	GLU
1	D	18	ILE
1	D	20	PRO
1	D	21	GLU
1	D	24	LYS
1	D	29	LEU
1	D	70	VAL
1	D	81	GLU
1	D	109	VAL
1	D	114	LYS
1	D	124	LEU
1	D	129	SER
1	D	134	MET

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Mol	Chain	Res	Type
1	D	136	ILE
1	D	137	LEU
1	D	170	VAL
1	D	176	LEU
1	D	192	LYS
1	D	199	MET
1	D	207	THR
1	D	208	LYS
1	D	221	VAL
1	D	241	GLU
1	D	249	GLU
1	D	252	LEU
1	D	255	LEU
1	D	268	PRO
1	D	322	ASN
1	D	346	HIS
1	D	350	ASP
1	D	351	THR
1	D	354	LEU
1	D	355	VAL
1	D	356	MET
1	D	362	THR
1	D	368	VAL
1	D	371	ASP
1	E	21	GLU
1	E	95	VAL
1	E	96	LEU
1	E	104	THR
1	E	105	ASN
1	E	127	ARG
1	E	132	GLN
1	E	134	MET
1	E	147	ARG
1	E	176	LEU
1	E	207	THR
1	E	210	GLN
1	E	241	GLU
1	E	242	GLU
1	E	244	ARG
1	E	252	LEU
1	E	253	LYS
1	E	258	THR

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Mol	Chain	Res	Type
1	E	270	LYS
1	E	330	ASP
1	E	346	HIS
1	E	348	ASP
1	E	349	LYS
1	E	350	ASP
2	F	298	GLU
2	F	318	MET
2	F	324	GLN
2	F	342	SER
2	F	364	ASN
2	F	367	TYR
2	F	374	GLU
2	F	384	ASP
2	F	420	THR
1	G	10	ARG
1	G	27	VAL
1	G	31	PHE
1	G	41	VAL
1	G	60	THR
1	G	92	GLU
1	G	164	MET
1	G	170	VAL
1	G	176	LEU
1	G	177	VAL
1	G	192	LYS
1	G	198	VAL
1	G	199	MET
1	G	220	THR
1	G	222	ASP
1	G	252	LEU
1	G	255	LEU
1	G	270	LYS
1	G	308	LYS
1	G	311	VAL
1	G	352	LYS
1	G	361	GLU
1	G	362	THR
1	G	369	THR
1	H	1	MET
1	H	10	ARG
1	H	15	ARG

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Mol	Chain	Res	Type
1	H	25	LYS
1	H	26	LEU
1	H	35	VAL
1	H	37	GLN
1	H	59	SER
1	H	67	GLN
1	H	72	TRP
1	H	76	ARG
1	H	97	MET
1	H	105	ASN
1	H	112	LEU
1	H	125	MET
1	H	147	ARG
1	H	158	ARG
1	H	160	PHE
1	H	164	MET
1	H	170	VAL
1	H	176	LEU
1	H	192	LYS
1	H	194	LEU
1	H	244	ARG
1	H	247	GLN
1	H	252	LEU
1	H	277	THR
1	H	278	GLU
1	H	279	GLU
1	H	330	ASP
1	H	334	LEU
1	H	339	LEU
1	H	342	PHE
1	H	344	THR
1	H	352	LYS
1	H	354	LEU
1	H	356	MET
2	I	334	LEU
2	I	348	VAL
2	I	358	VAL
2	I	376	ILE
2	I	384	ASP
2	I	422	LEU
2	I	425	LYS
2	I	439	LEU

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Mol	Chain	Res	Type
2	I	451	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	247	GLN
1	A	322	ASN
1	A	376	HIS
1	B	99	HIS
1	B	105	ASN
1	B	142	ASN
1	B	186	GLN
1	B	210	GLN
1	B	247	GLN
1	B	320	HIS
1	B	376	HIS
2	C	322	GLN
2	C	325	HIS
2	C	364	ASN
2	C	443	ASN
2	C	444	ASN
2	C	458	GLN
2	C	464	ASN
1	D	75	GLN
1	D	99	HIS
1	D	105	ASN
1	D	186	GLN
1	D	210	GLN
1	D	247	GLN
1	D	300	ASN
1	D	320	HIS
1	D	322	ASN
1	D	338	ASN
1	D	346	HIS
1	D	376	HIS
1	E	63	GLN
1	E	132	GLN
1	E	142	ASN
1	E	186	GLN
1	E	341	ASN
2	F	324	GLN

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Mol	Chain	Res	Type
2	F	458	GLN
1	G	37	GLN
1	G	142	ASN
1	G	186	GLN
1	G	338	ASN
1	G	341	ASN
1	G	376	HIS
1	H	63	GLN
1	H	67	GLN
1	H	105	ASN
1	H	142	ASN
1	H	247	GLN
1	H	300	ASN
1	H	322	ASN
1	H	341	ASN
1	H	376	HIS
2	I	325	HIS
2	I	357	ASN
2	I	443	ASN
2	I	461	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

12 monosaccharides 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	GLC	J	1	3	11,11,12	1.25	1 (9%)	15,15,17	0.77	1 (6%)
3	FRU	J	2	3	11,12,12	1.46	2 (18%)	10,18,18	0.59	0
3	GLC	K	1	3	11,11,12	1.17	1 (9%)	15,15,17	0.91	1 (6%)
3	FRU	K	2	3	11,12,12	1.53	2 (18%)	10,18,18	0.65	0
3	GLC	L	1	3	11,11,12	1.29	1 (9%)	15,15,17	0.85	1 (6%)
3	FRU	L	2	3	11,12,12	1.53	2 (18%)	10,18,18	0.64	0
3	GLC	M	1	3	11,11,12	1.03	1 (9%)	15,15,17	0.84	1 (6%)
3	FRU	M	2	3	11,12,12	1.63	2 (18%)	10,18,18	0.71	0
3	GLC	N	1	3	11,11,12	1.37	1 (9%)	15,15,17	0.92	1 (6%)
3	FRU	N	2	3	11,12,12	1.67	3 (27%)	10,18,18	0.62	0
3	GLC	O	1	3	11,11,12	1.34	1 (9%)	15,15,17	0.84	1 (6%)
3	FRU	O	2	3	11,12,12	1.54	2 (18%)	10,18,18	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	J	1	3	-	2/2/19/22	0/1/1/1
3	FRU	J	2	3	-	0/5/24/24	0/1/1/1
3	GLC	K	1	3	-	1/2/19/22	0/1/1/1
3	FRU	K	2	3	-	2/5/24/24	0/1/1/1
3	GLC	L	1	3	-	2/2/19/22	0/1/1/1
3	FRU	L	2	3	-	0/5/24/24	0/1/1/1
3	GLC	M	1	3	-	0/2/19/22	0/1/1/1
3	FRU	M	2	3	-	0/5/24/24	0/1/1/1
3	GLC	N	1	3	-	2/2/19/22	0/1/1/1
3	FRU	N	2	3	-	2/5/24/24	0/1/1/1
3	GLC	O	1	3	-	2/2/19/22	0/1/1/1
3	FRU	O	2	3	-	2/5/24/24	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	FRU	C4-C5	-4.13	1.42	1.53
3	J	2	FRU	C4-C5	-3.91	1.43	1.53
3	L	2	FRU	C4-C5	-3.83	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	2	FRU	O2-C2	3.62	1.46	1.40
3	O	2	FRU	C4-C5	-3.54	1.44	1.53
3	N	1	GLC	O5-C1	3.52	1.49	1.43
3	K	2	FRU	O2-C2	3.48	1.46	1.40
3	N	2	FRU	C4-C5	-3.39	1.44	1.53
3	K	2	FRU	C4-C5	-3.38	1.44	1.53
3	O	1	GLC	O5-C1	3.26	1.48	1.43
3	L	1	GLC	O5-C1	3.17	1.48	1.43
3	O	2	FRU	O2-C2	3.15	1.46	1.40
3	K	1	GLC	O5-C1	3.12	1.48	1.43
3	J	1	GLC	O5-C1	3.09	1.48	1.43
3	M	2	FRU	O2-C2	3.00	1.45	1.40
3	L	2	FRU	O2-C2	2.98	1.45	1.40
3	M	1	GLC	O5-C1	2.78	1.48	1.43
3	J	2	FRU	O2-C2	2.56	1.45	1.40
3	N	2	FRU	C1-C2	2.12	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	1	GLC	C2-C3-C4	-2.46	106.64	110.89
3	O	1	GLC	C2-C3-C4	-2.39	106.76	110.89
3	L	1	GLC	C2-C3-C4	-2.39	106.76	110.89
3	N	1	GLC	C2-C3-C4	-2.38	106.77	110.89
3	J	1	GLC	C2-C3-C4	-2.37	106.80	110.89
3	K	1	GLC	C2-C3-C4	-2.24	107.02	110.89

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	2	FRU	C4-C5-C6-O6
3	K	2	FRU	O5-C5-C6-O6
3	N	1	GLC	O5-C5-C6-O6
3	N	2	FRU	C4-C5-C6-O6
3	N	2	FRU	O5-C5-C6-O6
3	N	1	GLC	C4-C5-C6-O6
3	O	1	GLC	C4-C5-C6-O6
3	O	2	FRU	O5-C5-C6-O6
3	J	1	GLC	C4-C5-C6-O6
3	L	1	GLC	C4-C5-C6-O6
3	O	2	FRU	C4-C5-C6-O6

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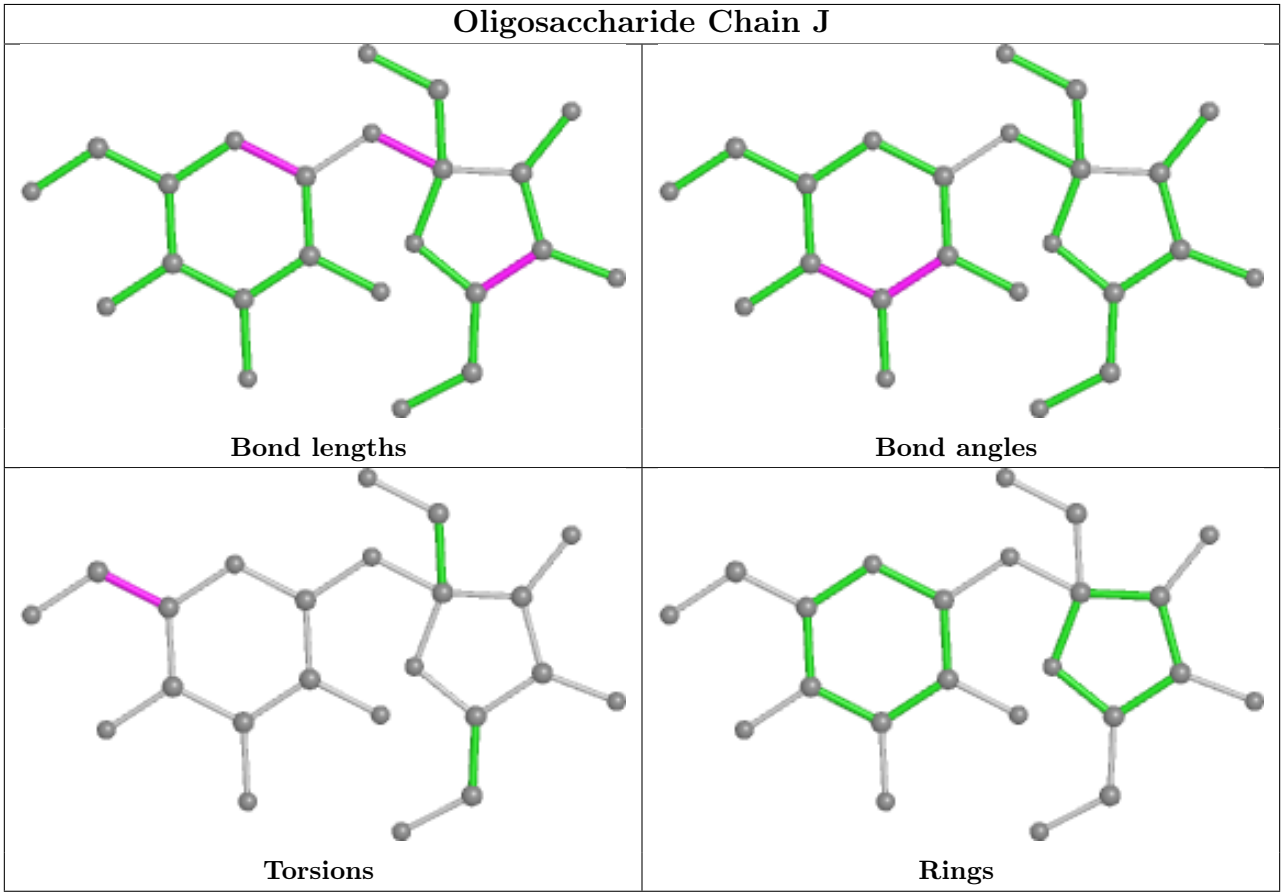
Mol	Chain	Res	Type	Atoms
3	O	1	GLC	O5-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
3	K	1	GLC	C4-C5-C6-O6
3	L	1	GLC	O5-C5-C6-O6

There are no ring outliers.

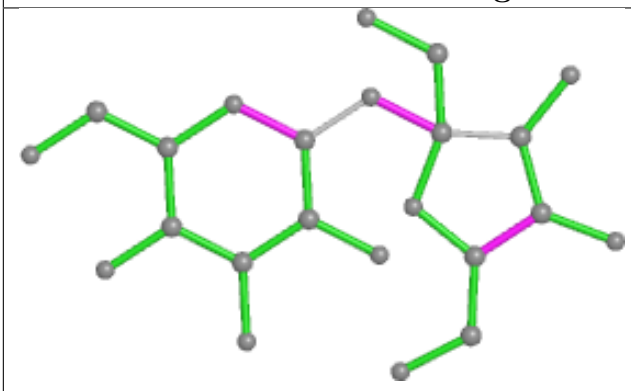
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	2	FRU	1	0
3	O	2	FRU	1	0

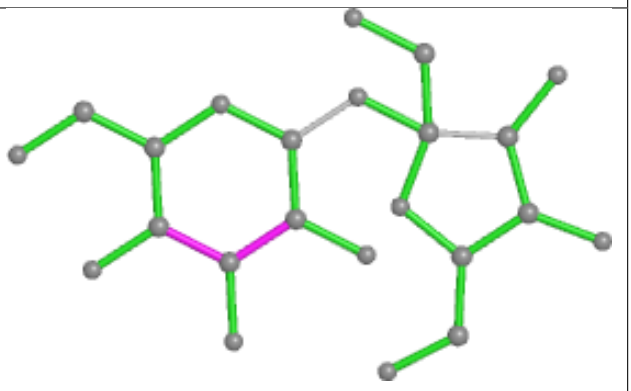
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



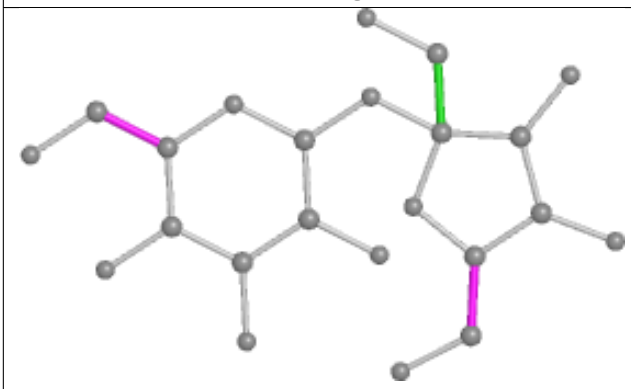
Oligosaccharide Chain K



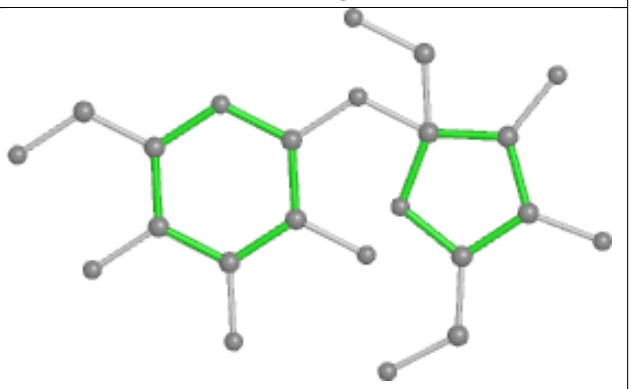
Bond lengths



Bond angles

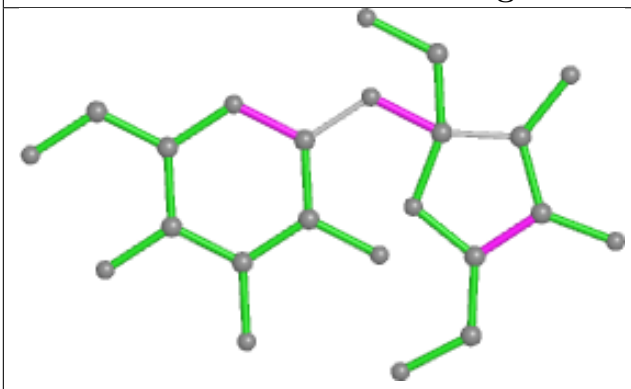


Torsions

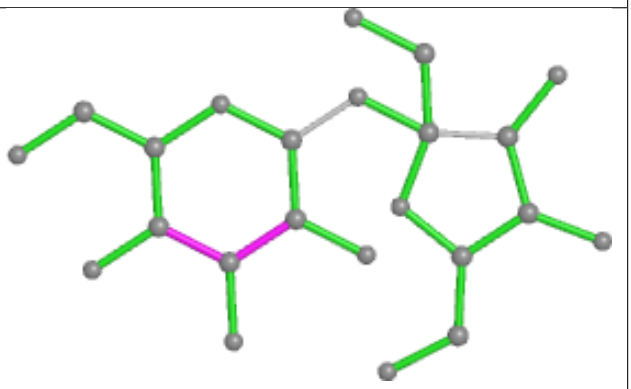


Rings

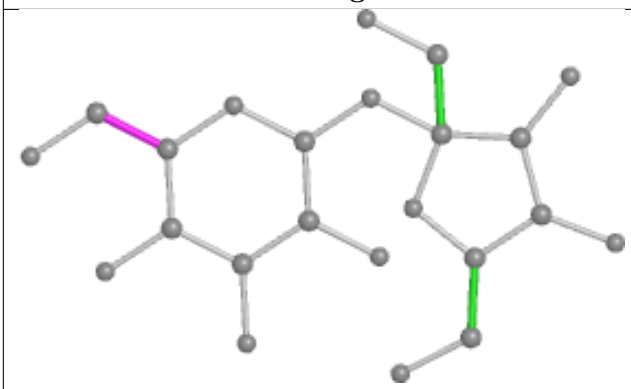
Oligosaccharide Chain L



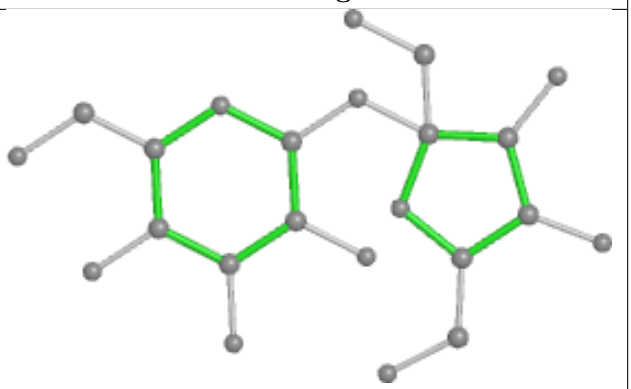
Bond lengths



Bond angles

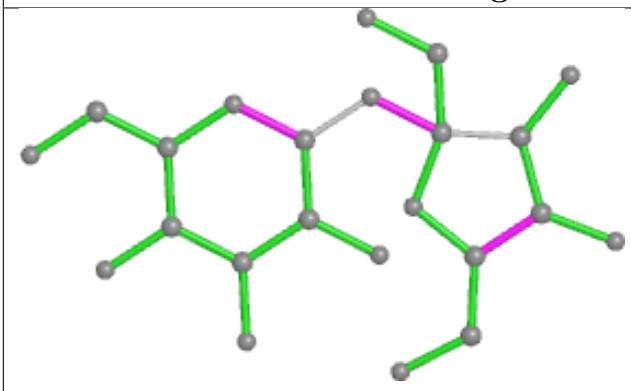


Torsions

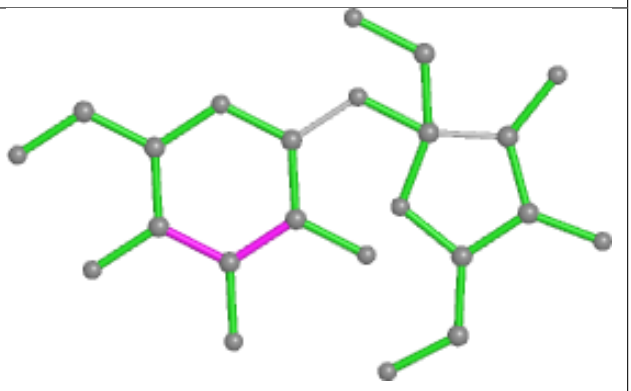


Rings

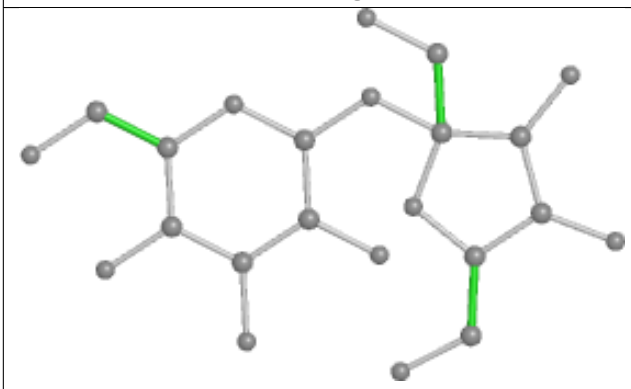
Oligosaccharide Chain M



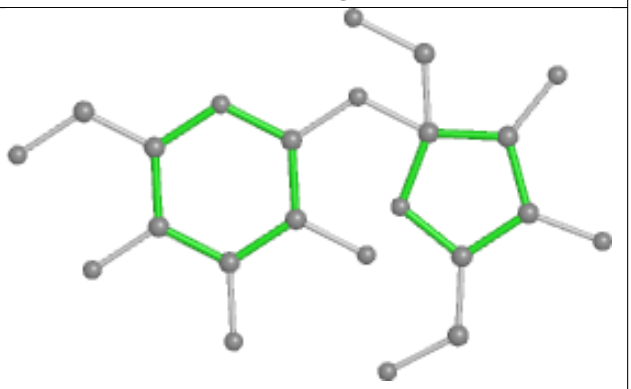
Bond lengths



Bond angles

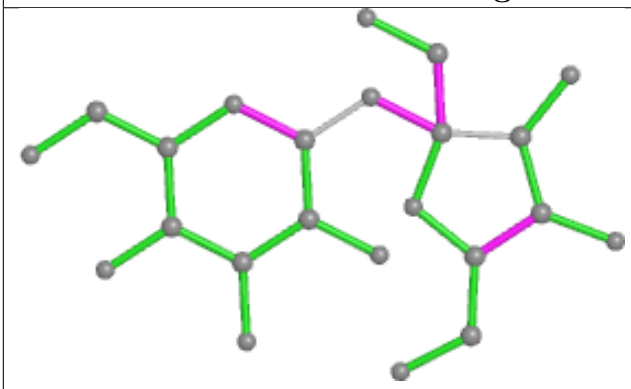


Torsions

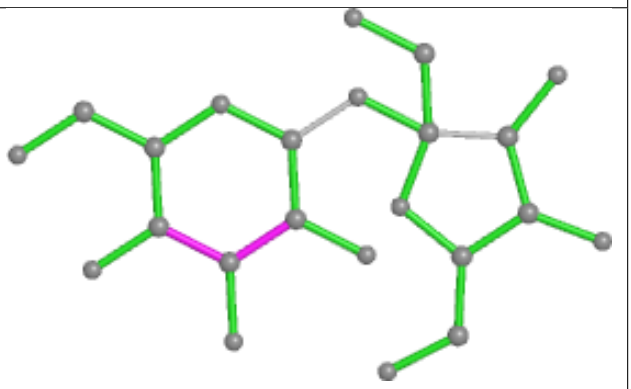


Rings

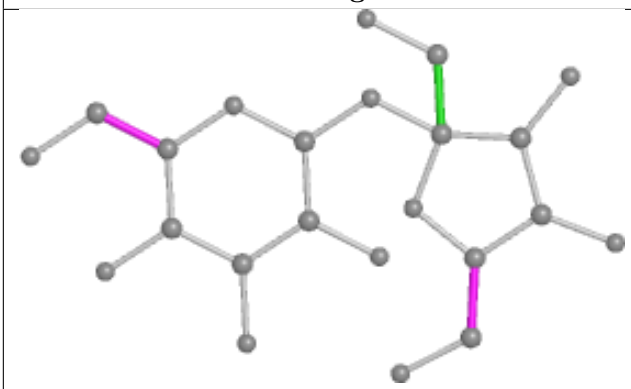
Oligosaccharide Chain N



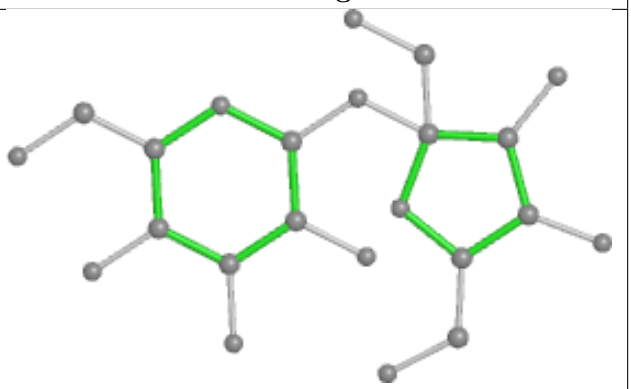
Bond lengths



Bond angles

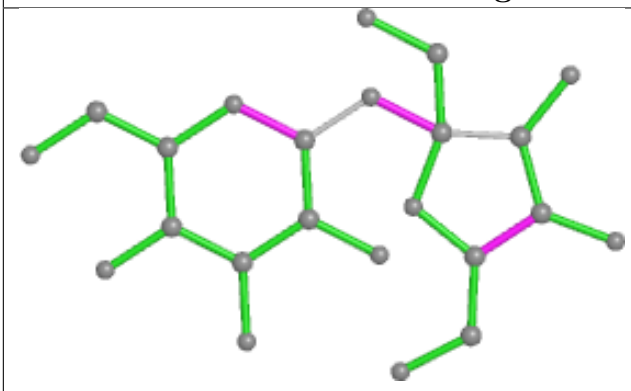


Torsions

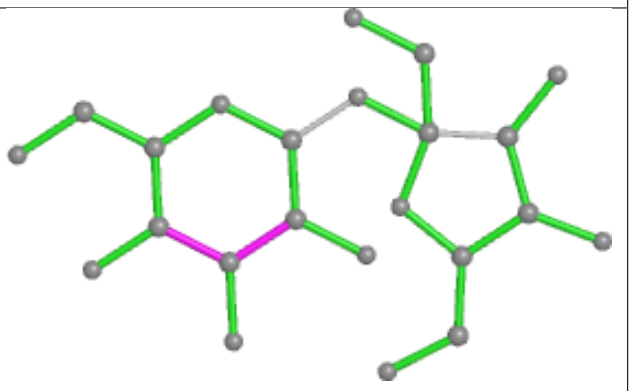


Rings

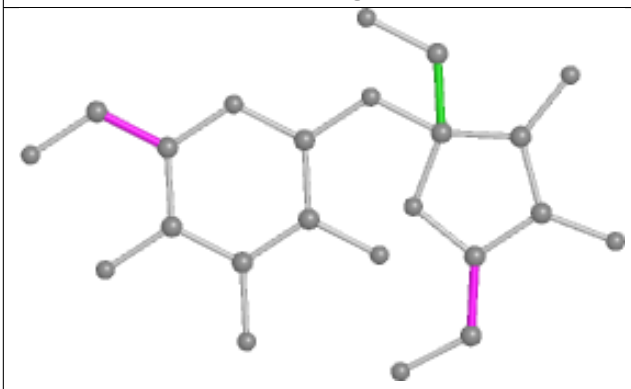
Oligosaccharide Chain O



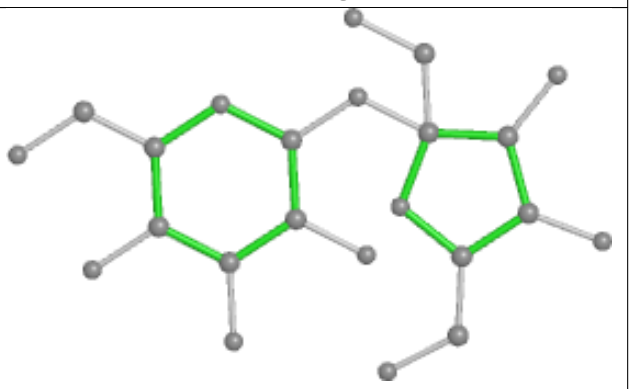
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAD	D	400	-	42,48,48	2.47	14 (33%)	50,73,73	2.26	20 (40%)
6	NDP	F	500	-	45,52,52	2.05	13 (28%)	53,80,80	1.95	17 (32%)
4	NAD	H	400	-	42,48,48	2.47	15 (35%)	50,73,73	2.27	17 (34%)
4	NAD	B	400	-	42,48,48	2.75	19 (45%)	50,73,73	2.64	17 (34%)
6	NDP	I	500	-	45,52,52	2.39	16 (35%)	53,80,80	2.04	18 (33%)
4	NAD	G	400	-	42,48,48	2.55	14 (33%)	50,73,73	2.82	21 (42%)
6	NDP	C	500	-	45,52,52	2.02	15 (33%)	53,80,80	2.02	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAD	A	400	-	42,48,48	2.58	18 (42%)	50,73,73	2.49	21 (42%)

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
4	NAD	D	400	-	-	9/26/62/62	0/5/5/5
6	NDP	F	500	-	-	14/30/77/77	0/5/5/5
4	NAD	H	400	-	-	11/26/62/62	0/5/5/5
4	NAD	B	400	-	-	16/26/62/62	0/5/5/5
6	NDP	I	500	-	-	13/30/77/77	0/5/5/5
4	NAD	G	400	-	-	8/26/62/62	0/5/5/5
6	NDP	C	500	-	-	12/30/77/77	0/5/5/5
4	NAD	A	400	-	-	15/26/62/62	0/5/5/5

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	500	NDP	O4D-C1D	8.19	1.61	1.42
4	B	400	NAD	O4B-C1B	7.74	1.51	1.41
4	H	400	NAD	O4B-C1B	7.44	1.51	1.41
4	A	400	NAD	O4B-C1B	7.32	1.51	1.41
4	D	400	NAD	O4B-C1B	7.20	1.51	1.41
4	B	400	NAD	C2N-N1N	7.14	1.43	1.35
4	G	400	NAD	C2N-N1N	7.02	1.43	1.35
4	G	400	NAD	O4B-C1B	6.81	1.50	1.41
4	A	400	NAD	C2N-N1N	6.50	1.42	1.35
6	I	500	NDP	O4B-C1B	6.29	1.49	1.41
6	C	500	NDP	O4B-C1B	6.19	1.49	1.41
6	F	500	NDP	O4B-C1B	5.85	1.49	1.41
4	D	400	NAD	C2N-N1N	5.54	1.41	1.35
4	H	400	NAD	C2N-N1N	5.52	1.41	1.35
4	G	400	NAD	C2B-C1B	-5.31	1.45	1.53
4	A	400	NAD	O4D-C1D	5.15	1.48	1.41
4	H	400	NAD	C2B-C1B	-5.10	1.46	1.53
4	B	400	NAD	C6N-N1N	4.83	1.47	1.35
4	G	400	NAD	C6N-N1N	4.78	1.47	1.35
4	B	400	NAD	C2B-C1B	-4.71	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	400	NAD	C5A-C4A	4.57	1.53	1.40
4	A	400	NAD	C2B-C1B	-4.57	1.46	1.53
4	G	400	NAD	C2N-C3N	4.56	1.46	1.39
4	H	400	NAD	C6N-N1N	4.48	1.46	1.35
4	B	400	NAD	C2N-C3N	4.38	1.45	1.39
4	D	400	NAD	C6N-N1N	4.35	1.46	1.35
4	H	400	NAD	PN-O5D	-4.33	1.41	1.59
4	H	400	NAD	C5A-C4A	4.27	1.52	1.40
4	B	400	NAD	O4D-C1D	4.26	1.47	1.41
4	G	400	NAD	C5A-C4A	4.26	1.52	1.40
4	B	400	NAD	C5A-C4A	4.25	1.52	1.40
6	I	500	NDP	C5A-C4A	4.24	1.52	1.40
6	F	500	NDP	C5A-C4A	4.10	1.51	1.40
4	D	400	NAD	C2B-C1B	-4.07	1.47	1.53
4	D	400	NAD	O4D-C1D	4.03	1.46	1.41
6	F	500	NDP	C4N-C5N	-4.03	1.38	1.48
4	A	400	NAD	C6N-N1N	4.02	1.45	1.35
4	A	400	NAD	C5A-C4A	3.99	1.51	1.40
4	A	400	NAD	C2N-C3N	3.87	1.45	1.39
6	I	500	NDP	C4N-C5N	-3.82	1.38	1.48
6	I	500	NDP	C2N-C3N	3.71	1.45	1.34
4	D	400	NAD	C2N-C3N	3.67	1.44	1.39
4	D	400	NAD	C4N-C3N	3.63	1.45	1.39
6	F	500	NDP	C2N-C3N	3.60	1.45	1.34
6	C	500	NDP	C4N-C5N	-3.58	1.39	1.48
4	B	400	NAD	C2D-C1D	3.56	1.59	1.53
6	F	500	NDP	C4N-C3N	-3.47	1.43	1.49
4	H	400	NAD	C2N-C3N	3.47	1.44	1.39
6	C	500	NDP	C5A-C4A	3.37	1.49	1.40
6	F	500	NDP	C2D-C1D	3.34	1.64	1.53
4	D	400	NAD	C2A-N1A	3.29	1.40	1.33
6	I	500	NDP	C4N-C3N	-3.21	1.43	1.49
4	G	400	NAD	C4N-C3N	3.18	1.44	1.39
4	B	400	NAD	C4N-C3N	3.18	1.44	1.39
4	H	400	NAD	C4N-C3N	3.18	1.44	1.39
4	B	400	NAD	PN-O2N	3.17	1.70	1.55
6	C	500	NDP	C6N-N1N	3.13	1.45	1.37
6	F	500	NDP	C3B-C4B	-3.12	1.45	1.53
6	I	500	NDP	C6N-C5N	3.12	1.38	1.33
6	C	500	NDP	C4N-C3N	-3.11	1.43	1.49
6	C	500	NDP	C6N-C5N	3.06	1.38	1.33
6	C	500	NDP	C2N-C3N	3.06	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	500	NDP	C3B-C2B	-3.05	1.46	1.52
6	I	500	NDP	C6N-N1N	3.05	1.44	1.37
4	G	400	NAD	C2D-C1D	-3.03	1.49	1.53
6	I	500	NDP	C3B-C2B	-2.99	1.46	1.52
4	G	400	NAD	C2A-N1A	2.95	1.39	1.33
6	C	500	NDP	P2B-O3X	-2.92	1.43	1.54
4	D	400	NAD	C3B-C4B	-2.87	1.45	1.53
4	H	400	NAD	C2A-N1A	2.86	1.39	1.33
6	F	500	NDP	C6N-N1N	2.83	1.44	1.37
6	I	500	NDP	C2A-N1A	2.81	1.39	1.33
4	G	400	NAD	O2B-C2B	-2.73	1.36	1.43
6	C	500	NDP	O4D-C1D	2.73	1.48	1.42
4	B	400	NAD	C2D-C3D	2.71	1.60	1.53
4	D	400	NAD	O2B-C2B	-2.70	1.36	1.43
4	B	400	NAD	C2A-N1A	2.70	1.38	1.33
4	A	400	NAD	C2D-C3D	2.69	1.60	1.53
4	A	400	NAD	PN-O5D	-2.65	1.48	1.59
6	F	500	NDP	C6N-C5N	2.65	1.38	1.33
6	I	500	NDP	C2A-N3A	2.64	1.36	1.32
4	A	400	NAD	C2A-N1A	2.61	1.38	1.33
4	D	400	NAD	C2A-N3A	2.61	1.36	1.32
4	A	400	NAD	C2D-C1D	2.61	1.57	1.53
4	G	400	NAD	C2A-N3A	2.60	1.36	1.32
6	C	500	NDP	C3B-C4B	-2.60	1.46	1.53
4	H	400	NAD	C2A-N3A	2.58	1.36	1.32
4	G	400	NAD	C3B-C4B	-2.57	1.46	1.53
6	I	500	NDP	P2B-O3X	-2.54	1.45	1.54
6	F	500	NDP	C3B-C2B	-2.53	1.47	1.52
4	A	400	NAD	C4N-C3N	2.50	1.43	1.39
6	F	500	NDP	C2A-N1A	2.49	1.38	1.33
4	B	400	NAD	O2B-C2B	-2.49	1.37	1.43
6	F	500	NDP	P2B-O3X	-2.48	1.45	1.54
4	B	400	NAD	O5B-C5B	-2.46	1.35	1.44
4	A	400	NAD	PN-O2N	-2.44	1.43	1.55
4	H	400	NAD	O2B-C2B	-2.43	1.37	1.43
6	C	500	NDP	C1D-N1N	2.42	1.53	1.46
6	I	500	NDP	C3B-C4B	-2.42	1.46	1.53
4	G	400	NAD	C2D-C3D	2.40	1.59	1.53
4	A	400	NAD	O2B-C2B	-2.40	1.37	1.43
4	D	400	NAD	C2B-C3B	-2.39	1.46	1.53
4	A	400	NAD	C2A-N3A	2.36	1.35	1.32
4	G	400	NAD	C2B-C3B	-2.36	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	NAD	C2B-C3B	-2.36	1.46	1.53
6	I	500	NDP	P2B-O2X	-2.34	1.45	1.54
6	I	500	NDP	O2B-C2B	-2.27	1.35	1.44
4	D	400	NAD	C2D-C1D	2.26	1.57	1.53
6	C	500	NDP	C2A-N1A	2.24	1.38	1.33
4	H	400	NAD	C2B-C3B	-2.24	1.47	1.53
4	A	400	NAD	O3B-C3B	2.23	1.48	1.43
4	H	400	NAD	O3D-C3D	2.23	1.48	1.43
4	A	400	NAD	PN-O1N	-2.21	1.43	1.50
4	H	400	NAD	C3B-C4B	-2.19	1.47	1.53
4	B	400	NAD	C2A-N3A	2.18	1.35	1.32
6	C	500	NDP	O3B-C3B	2.17	1.48	1.43
6	F	500	NDP	P2B-O2X	-2.14	1.46	1.54
6	C	500	NDP	O2B-C2B	-2.13	1.36	1.44
4	A	400	NAD	O3D-C3D	2.11	1.47	1.43
4	B	400	NAD	C3B-C4B	-2.10	1.47	1.53
4	B	400	NAD	C5B-C4B	-2.08	1.45	1.51
4	B	400	NAD	C5D-C4D	-2.04	1.45	1.51
4	H	400	NAD	C2D-C3D	2.02	1.58	1.53
6	I	500	NDP	O2D-C2D	-2.01	1.38	1.43

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	400	NAD	O5D-C5D-C4D	9.82	142.78	108.99
4	B	400	NAD	O4B-C4B-C5B	8.58	137.60	109.37
4	B	400	NAD	C6N-N1N-C2N	-8.28	114.42	121.97
4	G	400	NAD	C6N-N1N-C2N	-7.62	115.02	121.97
4	A	400	NAD	C6N-N1N-C2N	-7.47	115.17	121.97
4	H	400	NAD	C6N-N1N-C2N	-6.90	115.68	121.97
4	D	400	NAD	C6N-N1N-C2N	-6.85	115.73	121.97
4	B	400	NAD	O5D-C5D-C4D	5.91	129.33	108.99
4	G	400	NAD	O4D-C1D-C2D	5.59	115.10	106.93
4	H	400	NAD	O4D-C4D-C3D	5.23	115.47	105.11
4	A	400	NAD	O4D-C4D-C3D	4.83	114.68	105.11
4	A	400	NAD	O2B-C2B-C3B	4.77	127.26	111.82
4	D	400	NAD	O4D-C4D-C3D	4.72	114.46	105.11
4	B	400	NAD	C2B-C3B-C4B	4.68	111.74	102.64
4	H	400	NAD	O2B-C2B-C3B	4.59	126.68	111.82
4	G	400	NAD	O4D-C4D-C3D	4.55	114.12	105.11
6	C	500	NDP	O5B-C5B-C4B	4.55	124.65	108.99
4	B	400	NAD	O2B-C2B-C3B	4.50	126.39	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	500	NDP	C2D-C1D-N1N	4.48	124.53	113.30
6	I	500	NDP	O5B-C5B-C4B	4.46	124.34	108.99
4	A	400	NAD	O5D-C5D-C4D	4.44	124.28	108.99
6	F	500	NDP	C2B-C3B-C4B	4.40	111.55	101.99
6	F	500	NDP	O5D-C5D-C4D	4.37	124.04	108.99
6	I	500	NDP	O4D-C4D-C3D	4.35	113.72	105.11
6	F	500	NDP	O5B-C5B-C4B	4.32	123.87	108.99
6	C	500	NDP	O5D-C5D-C4D	4.32	123.87	108.99
4	A	400	NAD	PN-O5D-C5D	4.31	146.98	121.68
6	C	500	NDP	O4D-C1D-N1N	-4.31	99.63	108.06
4	D	400	NAD	O5D-C5D-C4D	4.28	123.72	108.99
4	H	400	NAD	O5B-C5B-C4B	4.23	123.56	108.99
6	F	500	NDP	O4D-C4D-C3D	4.23	113.48	105.11
4	A	400	NAD	C3N-C7N-N7N	-4.23	112.68	117.75
4	G	400	NAD	C3N-C7N-N7N	-4.18	112.74	117.75
4	H	400	NAD	C2B-C3B-C4B	4.16	110.73	102.64
4	G	400	NAD	O2B-C2B-C3B	4.14	125.21	111.82
4	G	400	NAD	C2B-C3B-C4B	4.13	110.67	102.64
4	A	400	NAD	O5B-C5B-C4B	4.06	122.98	108.99
6	F	500	NDP	O2B-C2B-C3B	4.02	126.24	111.68
4	A	400	NAD	C2B-C3B-C4B	4.01	110.44	102.64
4	H	400	NAD	C3N-C7N-N7N	-3.99	112.96	117.75
4	G	400	NAD	O5B-C5B-C4B	3.98	122.68	108.99
6	C	500	NDP	C2B-C3B-C4B	3.86	110.39	101.99
6	I	500	NDP	C4D-O4D-C1D	-3.79	101.11	109.47
4	D	400	NAD	O2B-C2B-C3B	3.77	124.01	111.82
4	D	400	NAD	C2B-C3B-C4B	3.76	109.94	102.64
4	D	400	NAD	O5B-C5B-C4B	3.74	121.86	108.99
4	B	400	NAD	C3N-C7N-N7N	-3.71	113.30	117.75
4	H	400	NAD	O4D-C1D-C2D	3.64	112.24	106.93
6	I	500	NDP	O2B-C2B-C3B	3.56	124.59	111.68
4	D	400	NAD	O4B-C4B-C5B	3.55	121.04	109.37
4	A	400	NAD	N3A-C2A-N1A	-3.54	123.14	128.68
6	I	500	NDP	C2B-C3B-C4B	3.54	109.68	101.99
6	C	500	NDP	O4D-C4D-C3D	3.52	112.09	105.11
4	B	400	NAD	O4D-C4D-C3D	3.52	112.08	105.11
4	B	400	NAD	N3A-C2A-N1A	-3.50	123.21	128.68
4	G	400	NAD	PN-O5D-C5D	3.50	142.19	121.68
6	I	500	NDP	PN-O5D-C5D	-3.45	101.46	121.68
4	H	400	NAD	N3A-C2A-N1A	-3.41	123.36	128.68
6	F	500	NDP	O4D-C1D-N1N	-3.39	101.43	108.06
6	C	500	NDP	N3A-C2A-N1A	-3.37	123.41	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	500	NDP	O2B-C2B-C3B	3.37	123.89	111.68
6	I	500	NDP	C2D-C3D-C4D	-3.34	96.15	102.64
6	C	500	NDP	C2D-C3D-C4D	-3.34	96.16	102.64
4	G	400	NAD	N3A-C2A-N1A	-3.30	123.51	128.68
4	D	400	NAD	O3D-C3D-C4D	3.19	120.29	111.05
4	G	400	NAD	C5N-C6N-N1N	3.19	124.97	120.40
4	B	400	NAD	C5N-C6N-N1N	3.17	124.95	120.40
4	A	400	NAD	C5N-C6N-N1N	3.16	124.94	120.40
4	H	400	NAD	O3D-C3D-C4D	3.14	120.14	111.05
4	D	400	NAD	C3N-C7N-N7N	-3.13	114.00	117.75
6	I	500	NDP	N3A-C2A-N1A	-3.09	123.84	128.68
6	I	500	NDP	C3N-C7N-N7N	-3.05	112.25	117.67
6	F	500	NDP	N3A-C2A-N1A	-3.02	123.96	128.68
6	F	500	NDP	O3D-C3D-C4D	3.00	119.73	111.05
4	H	400	NAD	O4B-C4B-C5B	2.96	119.12	109.37
4	A	400	NAD	C2D-C3D-C4D	-2.93	96.94	102.64
6	I	500	NDP	O4B-C4B-C5B	2.93	119.00	109.37
4	A	400	NAD	O3D-C3D-C4D	2.93	119.51	111.05
4	G	400	NAD	O4B-C4B-C5B	2.90	118.91	109.37
4	D	400	NAD	C5N-C6N-N1N	2.87	124.52	120.40
4	G	400	NAD	O3D-C3D-C4D	2.86	119.31	111.05
4	G	400	NAD	PN-O3-PA	-2.85	123.04	132.83
4	H	400	NAD	C5N-C6N-N1N	2.84	124.48	120.40
6	C	500	NDP	C2D-C1D-N1N	2.84	120.41	113.30
4	B	400	NAD	C3B-C2B-C1B	2.82	105.22	100.98
6	C	500	NDP	O4B-C4B-C5B	2.81	118.63	109.37
4	D	400	NAD	N3A-C2A-N1A	-2.81	124.29	128.68
4	G	400	NAD	C5D-C4D-C3D	-2.72	104.98	115.18
4	A	400	NAD	C2N-C3N-C4N	2.70	121.32	118.26
4	B	400	NAD	O3D-C3D-C4D	2.69	118.84	111.05
6	I	500	NDP	O3D-C3D-C4D	2.69	118.83	111.05
6	C	500	NDP	O5D-PN-O1N	2.65	119.42	109.07
6	C	500	NDP	C4D-O4D-C1D	-2.63	103.66	109.47
6	F	500	NDP	O4B-C4B-C5B	2.57	117.83	109.37
6	F	500	NDP	O5D-PN-O1N	2.55	119.02	109.07
6	C	500	NDP	O4D-C4D-C5D	2.54	117.74	109.37
6	F	500	NDP	C4D-O4D-C1D	-2.53	103.89	109.47
4	A	400	NAD	O4B-C4B-C5B	2.52	117.68	109.37
4	H	400	NAD	C2N-C3N-C4N	2.46	121.04	118.26
6	C	500	NDP	O3D-C3D-C4D	2.46	118.15	111.05
6	F	500	NDP	C3N-C7N-N7N	-2.45	113.31	117.67
4	B	400	NAD	O5D-PN-O1N	2.43	118.58	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	400	NAD	O7N-C7N-N7N	2.43	126.03	122.58
4	A	400	NAD	PN-O3-PA	-2.41	124.56	132.83
4	A	400	NAD	O2D-C2D-C3D	2.41	119.61	111.82
4	A	400	NAD	PA-O5B-C5B	2.40	135.73	121.68
6	F	500	NDP	C3N-C2N-N1N	-2.38	119.70	123.10
4	D	400	NAD	C3D-C2D-C1D	2.37	104.55	100.98
4	D	400	NAD	O4B-C1B-C2B	-2.36	103.47	106.93
4	B	400	NAD	C2N-C3N-C4N	2.35	120.92	118.26
6	I	500	NDP	PN-O3-PA	-2.33	124.83	132.83
4	H	400	NAD	O7N-C7N-N7N	2.32	125.87	122.58
6	F	500	NDP	C2D-C3D-C4D	-2.28	98.21	102.64
4	A	400	NAD	O4B-C4B-C3B	-2.28	100.61	105.11
4	G	400	NAD	O4D-C4D-C5D	-2.26	101.93	109.37
6	I	500	NDP	O2D-C2D-C3D	2.25	119.09	111.82
4	B	400	NAD	PN-O5D-C5D	2.24	134.82	121.68
4	H	400	NAD	PA-O5B-C5B	2.24	134.79	121.68
4	D	400	NAD	O5D-PN-O1N	2.24	117.80	109.07
6	C	500	NDP	PN-O3-PA	-2.23	125.16	132.83
6	C	500	NDP	C2A-N1A-C6A	2.23	122.57	118.75
4	H	400	NAD	O5D-C5D-C4D	2.23	116.67	108.99
4	G	400	NAD	O4B-C4B-C3B	-2.23	100.70	105.11
6	I	500	NDP	C3D-C2D-C1D	2.23	105.66	101.43
4	D	400	NAD	O4B-C4B-C3B	-2.23	100.71	105.11
4	A	400	NAD	O4D-C4D-C5D	2.23	116.70	109.37
6	C	500	NDP	PN-O5D-C5D	2.22	134.68	121.68
4	B	400	NAD	C2A-N1A-C6A	2.22	122.55	118.75
4	D	400	NAD	O4D-C1D-C2D	2.21	110.15	106.93
4	G	400	NAD	C2N-C3N-C4N	2.21	120.76	118.26
4	H	400	NAD	C2A-N1A-C6A	2.20	122.51	118.75
4	D	400	NAD	C2D-C3D-C4D	-2.19	98.39	102.64
4	D	400	NAD	O4D-C4D-C5D	2.18	116.54	109.37
6	I	500	NDP	O4B-C4B-C3B	-2.17	100.82	105.11
4	H	400	NAD	O4B-C4B-C3B	-2.14	100.88	105.11
6	I	500	NDP	O4D-C1D-N1N	-2.14	103.87	108.06
6	F	500	NDP	PN-O5D-C5D	2.12	134.14	121.68
6	F	500	NDP	O4D-C4D-C5D	2.12	116.36	109.37
4	A	400	NAD	C2A-N1A-C6A	2.11	122.37	118.75
4	B	400	NAD	C2D-C3D-C4D	-2.11	98.55	102.64
6	F	500	NDP	C2A-N1A-C6A	2.10	122.35	118.75
6	C	500	NDP	O2D-C2D-C3D	2.09	118.59	111.82
6	C	500	NDP	O4B-C4B-C3B	-2.09	100.98	105.11
4	D	400	NAD	C2N-C3N-C4N	2.09	120.62	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	400	NAD	O2D-C2D-C3D	2.07	118.51	111.82
4	B	400	NAD	C3D-C2D-C1D	2.05	104.06	100.98
6	I	500	NDP	C3N-C2N-N1N	-2.04	120.19	123.10
4	G	400	NAD	C2A-N1A-C6A	2.03	122.22	118.75
6	C	500	NDP	O2A-PA-O1A	2.02	122.24	112.24
4	G	400	NAD	PA-O5B-C5B	2.02	133.54	121.68
4	D	400	NAD	PN-O5D-C5D	2.00	133.43	121.68

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	400	NAD	PN-O3-PA-O5B
4	A	400	NAD	O4B-C4B-C5B-O5B
4	A	400	NAD	C5D-O5D-PN-O1N
4	A	400	NAD	O4D-C1D-N1N-C2N
4	A	400	NAD	O4D-C1D-N1N-C6N
4	A	400	NAD	C2D-C1D-N1N-C2N
4	A	400	NAD	C2D-C1D-N1N-C6N
4	B	400	NAD	C5B-O5B-PA-O1A
4	B	400	NAD	O4D-C4D-C5D-O5D
4	B	400	NAD	C2D-C1D-N1N-C2N
4	B	400	NAD	C2D-C1D-N1N-C6N
4	B	400	NAD	C2N-C3N-C7N-O7N
4	B	400	NAD	C2N-C3N-C7N-N7N
4	D	400	NAD	C5B-O5B-PA-O1A
4	D	400	NAD	C5B-O5B-PA-O3
4	D	400	NAD	PN-O3-PA-O5B
4	D	400	NAD	C5D-O5D-PN-O1N
4	D	400	NAD	O4D-C1D-N1N-C6N
4	G	400	NAD	C5B-O5B-PA-O1A
4	G	400	NAD	C5B-O5B-PA-O2A
4	H	400	NAD	C5B-O5B-PA-O1A
4	H	400	NAD	C5B-O5B-PA-O2A
4	H	400	NAD	C5D-O5D-PN-O3
4	H	400	NAD	C5D-O5D-PN-O1N
4	H	400	NAD	O4D-C1D-N1N-C2N
4	H	400	NAD	O4D-C1D-N1N-C6N
6	C	500	NDP	C1B-C2B-O2B-P2B
6	C	500	NDP	C5D-O5D-PN-O2N
6	C	500	NDP	O4D-C4D-C5D-O5D
6	C	500	NDP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
6	F	500	NDP	C5B-O5B-PA-O1A
6	F	500	NDP	C5D-O5D-PN-O2N
6	F	500	NDP	O4D-C4D-C5D-O5D
6	F	500	NDP	C2N-C3N-C7N-N7N
6	I	500	NDP	C5B-O5B-PA-O3
6	I	500	NDP	C2N-C3N-C7N-N7N
4	B	400	NAD	C4N-C3N-C7N-O7N
4	B	400	NAD	C4N-C3N-C7N-N7N
4	A	400	NAD	C3B-C4B-C5B-O5B
4	B	400	NAD	O4B-C4B-C5B-O5B
4	D	400	NAD	C3D-C4D-C5D-O5D
4	H	400	NAD	O4D-C4D-C5D-O5D
4	H	400	NAD	C3D-C4D-C5D-O5D
6	F	500	NDP	O4B-C4B-C5B-O5B
6	I	500	NDP	O4B-C4B-C5B-O5B
4	A	400	NAD	C2N-C3N-C7N-O7N
6	F	500	NDP	C1B-C2B-O2B-P2B
6	I	500	NDP	C1B-C2B-O2B-P2B
6	C	500	NDP	C2D-C1D-N1N-C6N
6	F	500	NDP	C2D-C1D-N1N-C6N
4	A	400	NAD	C2N-C3N-C7N-N7N
4	B	400	NAD	C3D-C4D-C5D-O5D
4	D	400	NAD	O4D-C4D-C5D-O5D
6	F	500	NDP	C3B-C4B-C5B-O5B
6	C	500	NDP	C3B-C2B-O2B-P2B
6	F	500	NDP	C3B-C2B-O2B-P2B
6	I	500	NDP	C3B-C2B-O2B-P2B
4	A	400	NAD	C4N-C3N-C7N-O7N
6	C	500	NDP	C2D-C1D-N1N-C2N
6	F	500	NDP	C2D-C1D-N1N-C2N
6	C	500	NDP	O4B-C4B-C5B-O5B
6	I	500	NDP	C3B-C4B-C5B-O5B
4	A	400	NAD	C4N-C3N-C7N-N7N
4	A	400	NAD	C4D-C5D-O5D-PN
4	H	400	NAD	C4B-C5B-O5B-PA
4	H	400	NAD	O4B-C4B-C5B-O5B
6	C	500	NDP	C3B-C4B-C5B-O5B
4	G	400	NAD	C4D-C5D-O5D-PN
4	B	400	NAD	C4D-C5D-O5D-PN
4	G	400	NAD	C4B-C5B-O5B-PA
4	B	400	NAD	PN-O3-PA-O5B
6	C	500	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
6	F	500	NDP	C2B-O2B-P2B-O1X
6	C	500	NDP	O4D-C1D-N1N-C2N
4	A	400	NAD	C5D-O5D-PN-O3
4	B	400	NAD	C5D-O5D-PN-O3
4	D	400	NAD	C5D-O5D-PN-O3
6	F	500	NDP	O4D-C1D-N1N-C6N
6	I	500	NDP	C5B-O5B-PA-O1A
6	I	500	NDP	C5B-O5B-PA-O2A
4	D	400	NAD	O4B-C4B-C5B-O5B
4	G	400	NAD	O4D-C4D-C5D-O5D
6	F	500	NDP	O4D-C1D-N1N-C2N
6	I	500	NDP	O4D-C1D-N1N-C6N
6	I	500	NDP	C2D-C1D-N1N-C6N
4	B	400	NAD	PN-O3-PA-O1A
4	A	400	NAD	O4D-C4D-C5D-O5D
4	G	400	NAD	C3D-C4D-C5D-O5D
6	C	500	NDP	C3D-C4D-C5D-O5D
4	B	400	NAD	C5B-O5B-PA-O3
4	G	400	NAD	C5B-O5B-PA-O3
4	H	400	NAD	C5B-O5B-PA-O3
6	F	500	NDP	C5B-O5B-PA-O3
4	B	400	NAD	PA-O3-PN-O1N
4	G	400	NAD	O4B-C4B-C5B-O5B
6	I	500	NDP	O4D-C4D-C5D-O5D
6	I	500	NDP	O4D-C1D-N1N-C2N
6	I	500	NDP	C2D-C1D-N1N-C2N

There are no ring outliers.

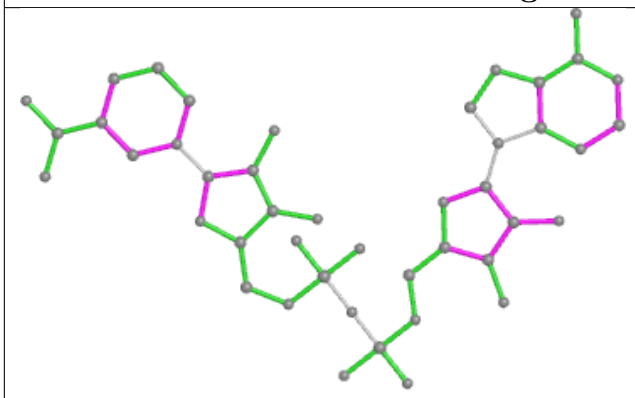
8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	400	NAD	3	0
6	F	500	NDP	10	0
4	H	400	NAD	8	0
4	B	400	NAD	9	0
6	I	500	NDP	3	0
4	G	400	NAD	6	0
6	C	500	NDP	4	0
4	A	400	NAD	2	0

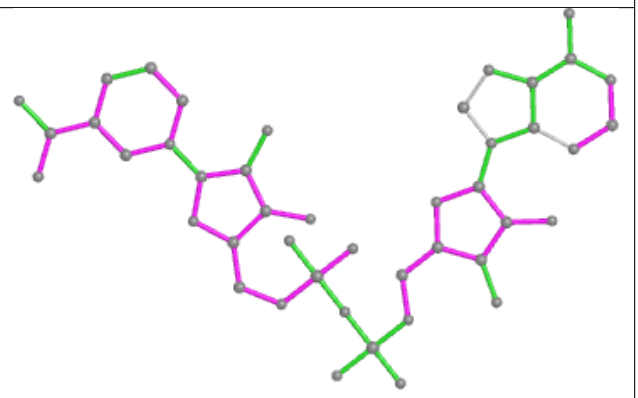
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

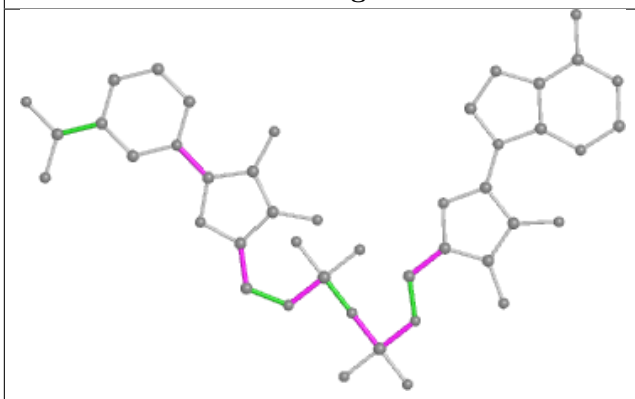
Ligand NAD D 400



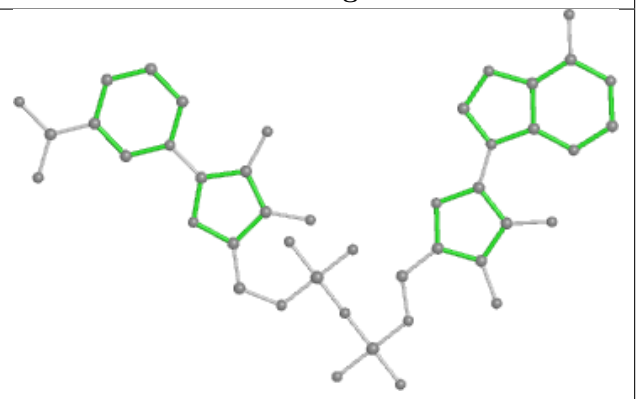
Bond lengths



Bond angles

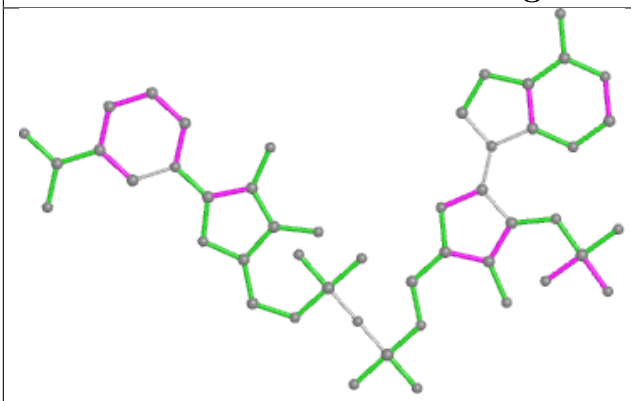


Torsions

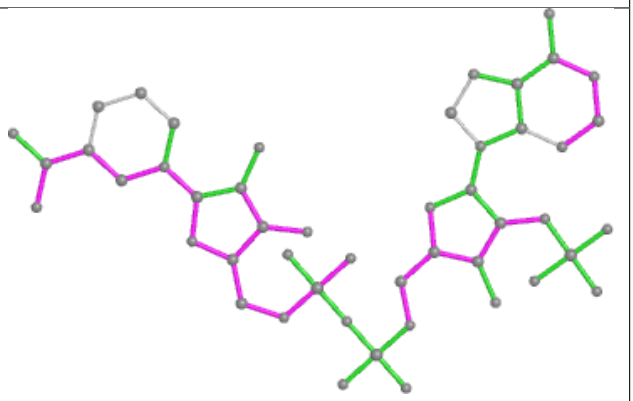


Rings

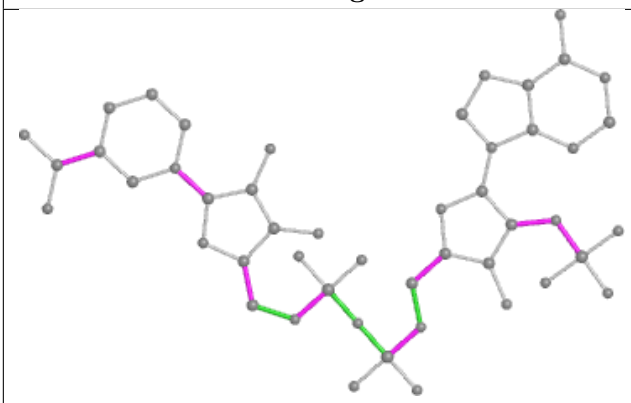
Ligand NDP F 500



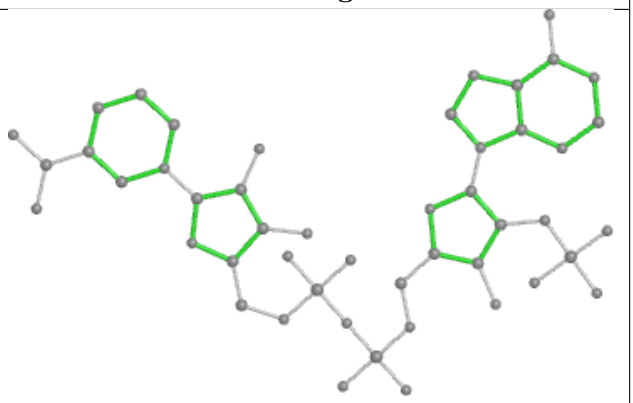
Bond lengths



Bond angles

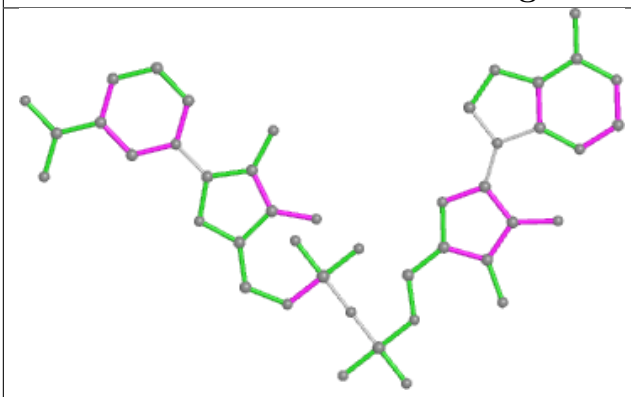


Torsions

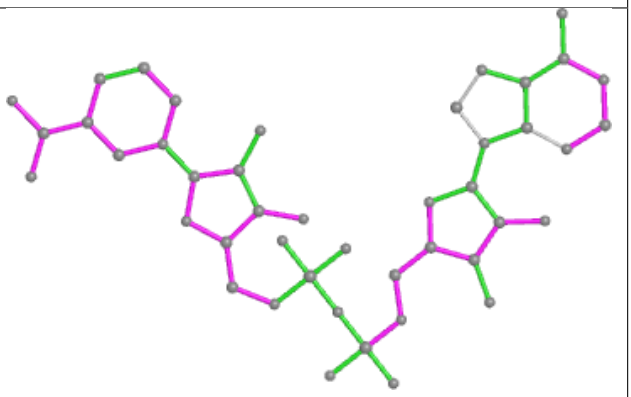


Rings

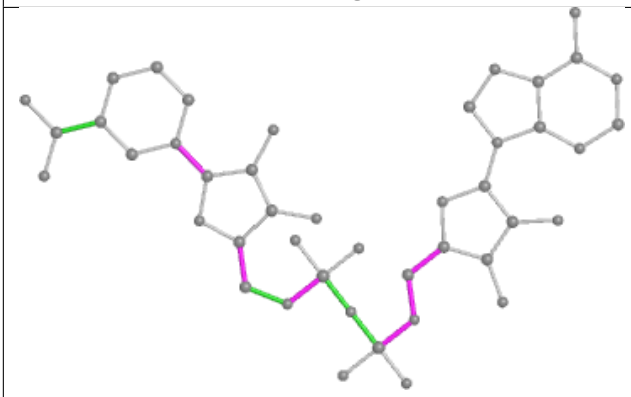
Ligand NAD H 400



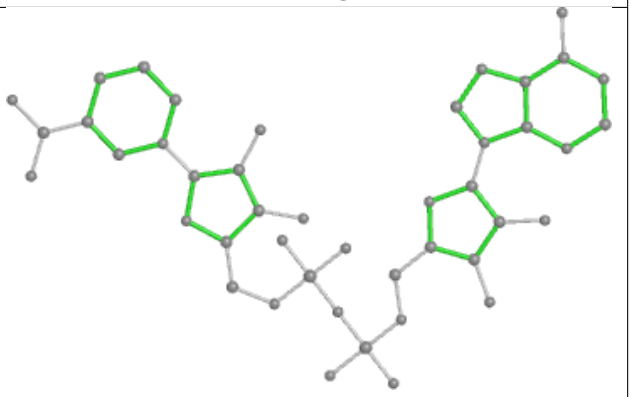
Bond lengths



Bond angles

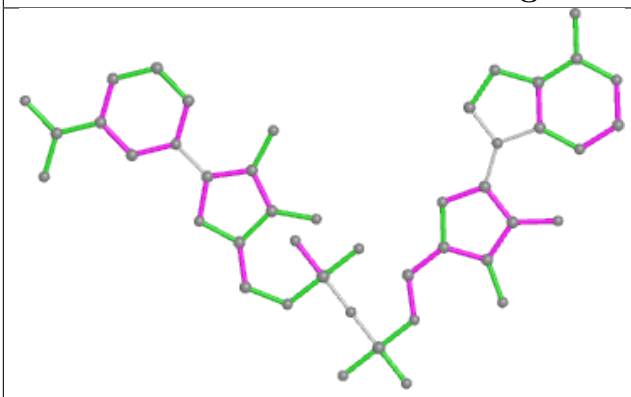


Torsions

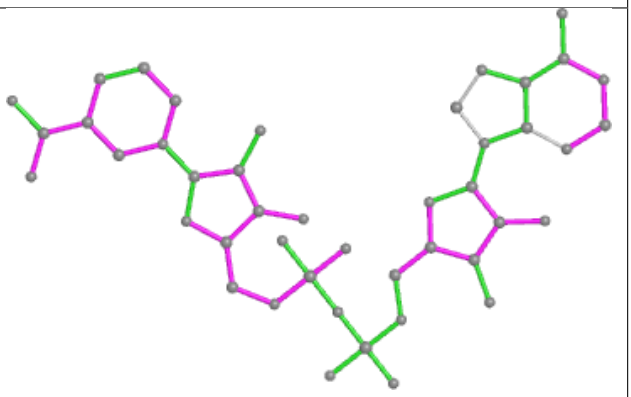


Rings

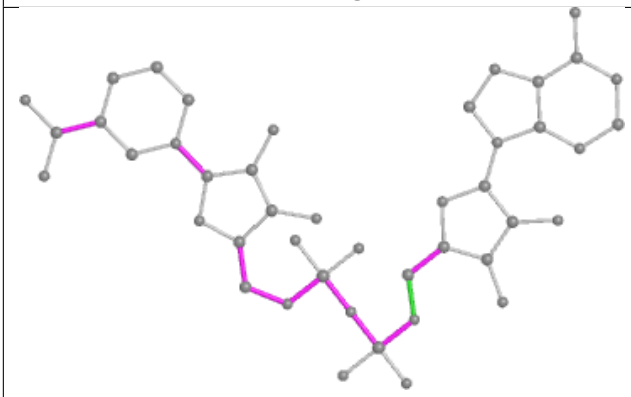
Ligand NAD B 400



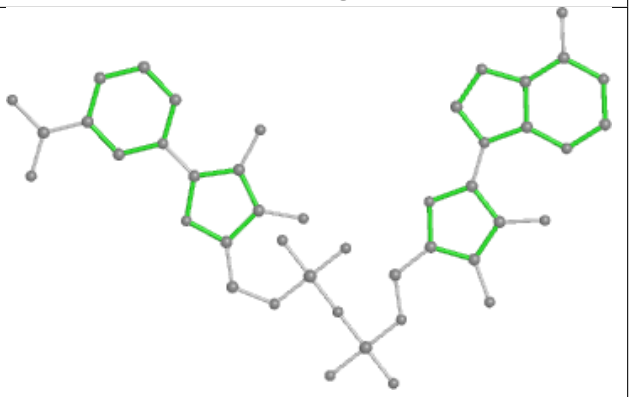
Bond lengths



Bond angles

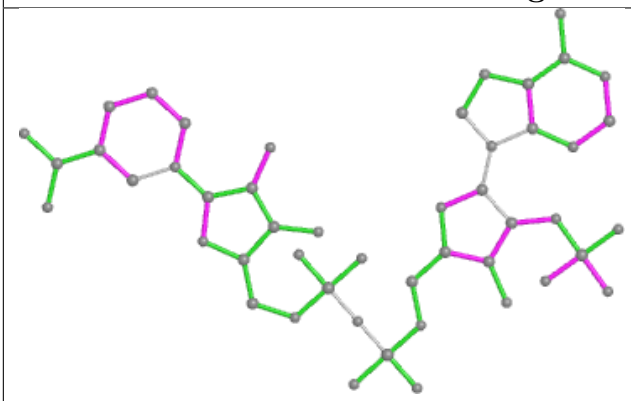


Torsions

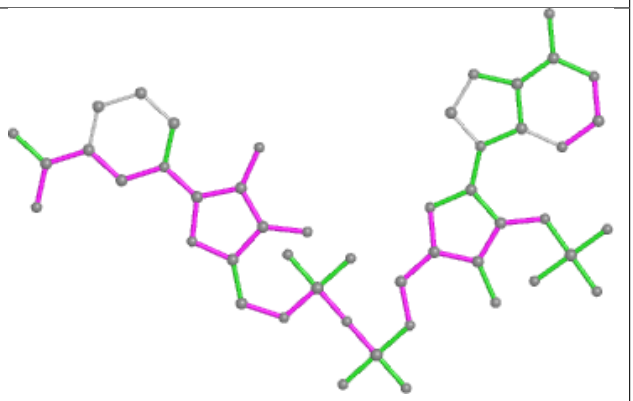


Rings

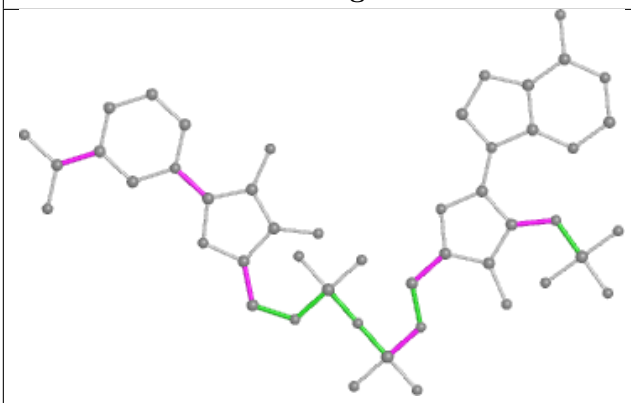
Ligand NDP I 500



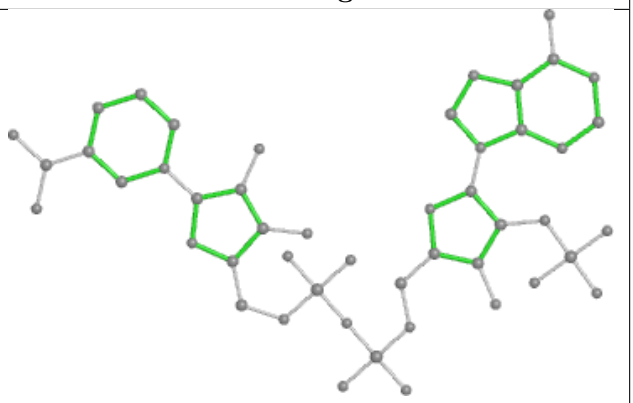
Bond lengths



Bond angles

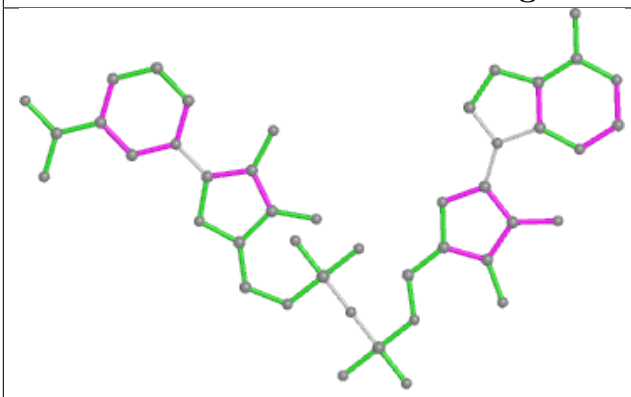


Torsions

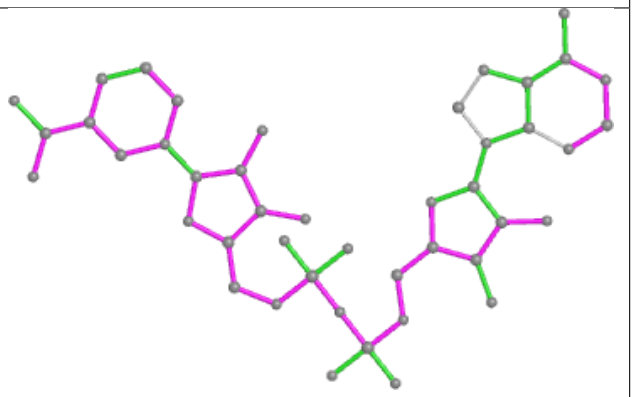


Rings

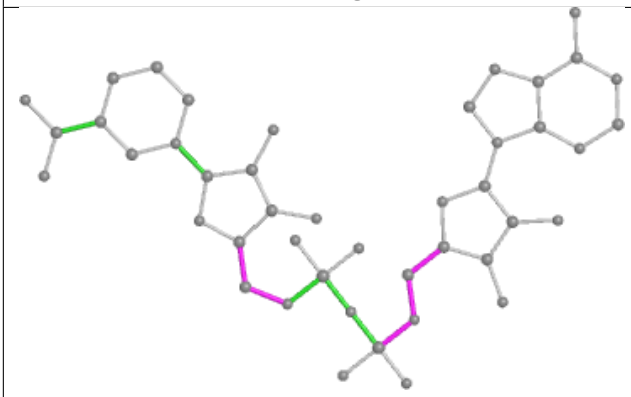
Ligand NAD G 400



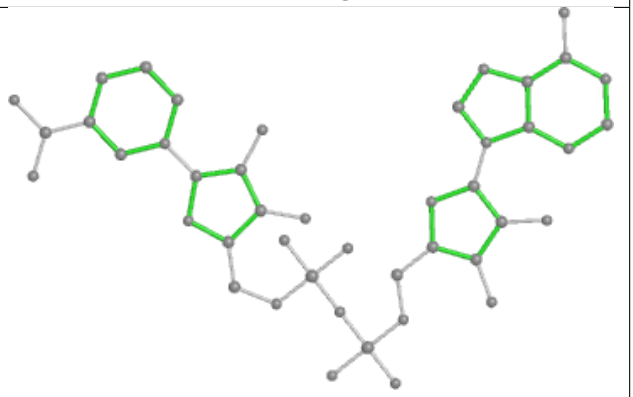
Bond lengths



Bond angles

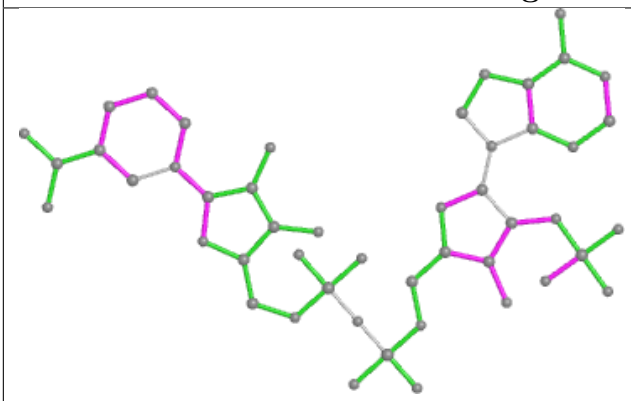


Torsions

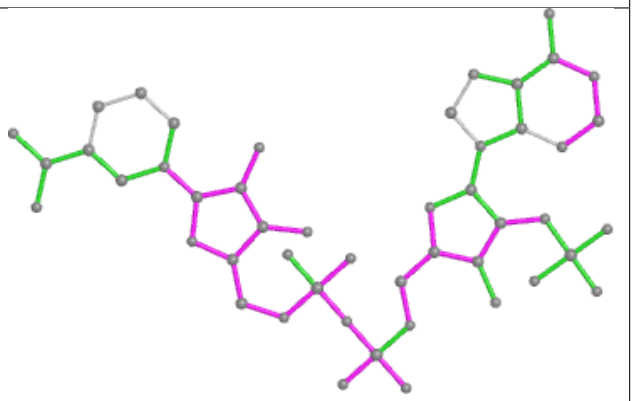


Rings

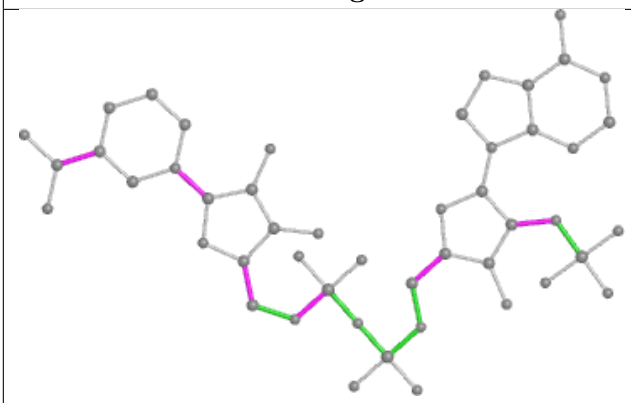
Ligand NDP C 500



Bond lengths



Bond angles



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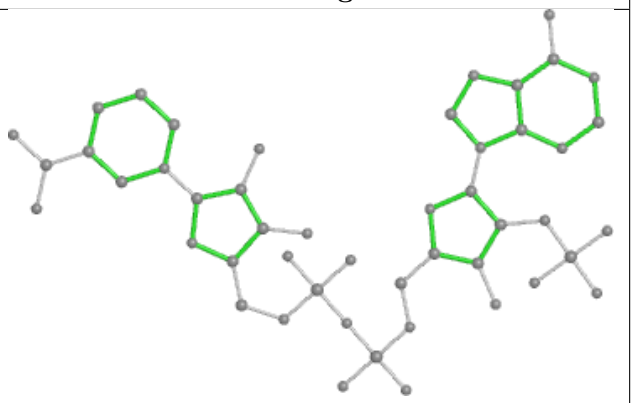
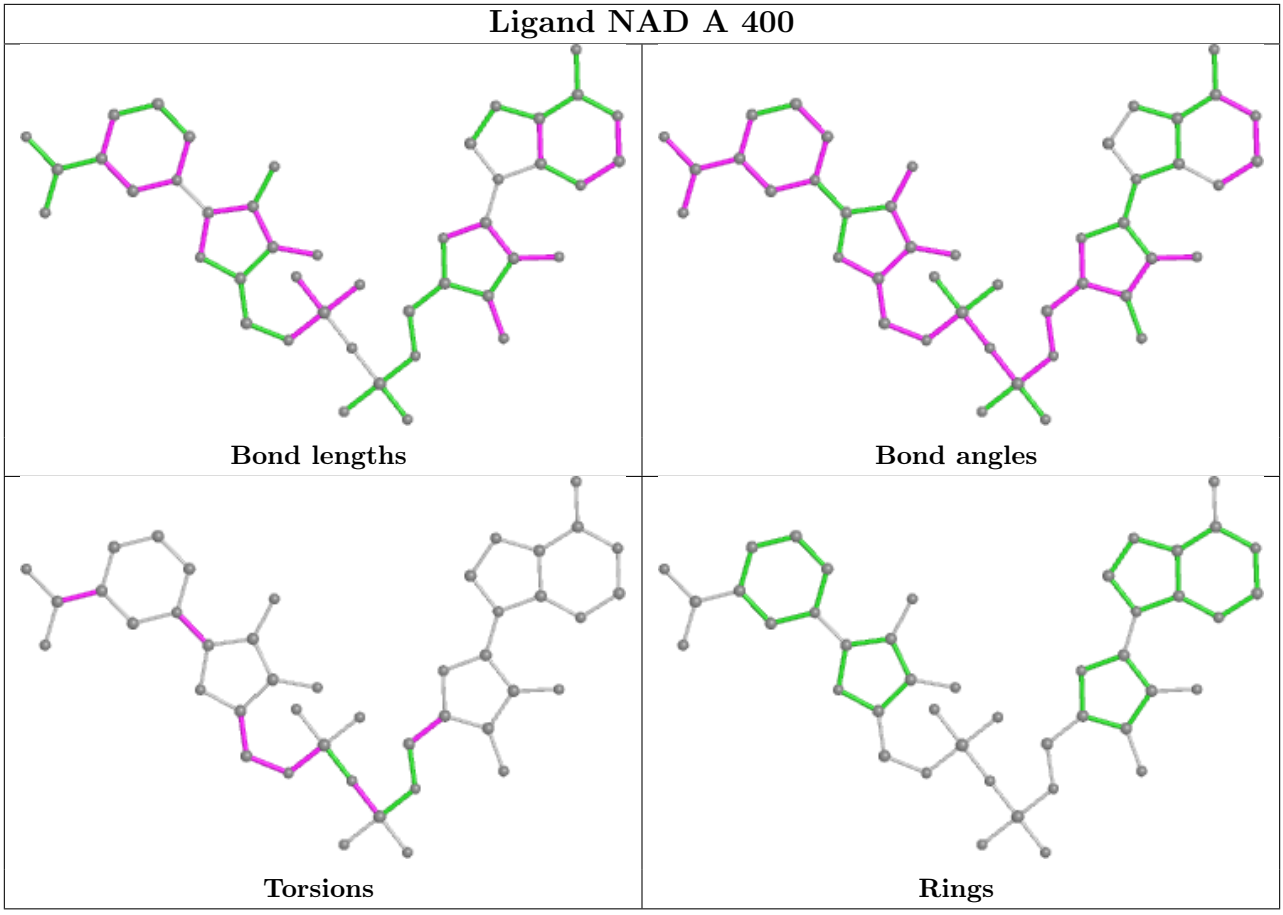


Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	343:LEU	C	344:THR	N	1.19

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	363/384 (94%)	-0.20	2 (0%) 89 78	30, 51, 77, 102	0
1	B	359/384 (93%)	-0.23	0 100 100	28, 52, 72, 98	0
1	D	378/384 (98%)	0.01	9 (2%) 59 37	36, 68, 94, 104	0
1	E	359/384 (93%)	-0.18	4 (1%) 80 64	33, 60, 79, 91	0
1	G	364/384 (94%)	-0.21	1 (0%) 94 88	35, 59, 84, 102	0
1	H	357/384 (92%)	0.06	10 (2%) 53 30	39, 72, 96, 104	0
2	C	174/174 (100%)	-0.39	0 100 100	32, 47, 61, 68	0
2	F	173/174 (99%)	-0.36	0 100 100	40, 52, 63, 75	0
2	I	173/174 (99%)	-0.27	0 100 100	42, 58, 73, 79	0
All	All	2700/2826 (95%)	-0.17	26 (0%) 82 67	28, 57, 90, 104	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.8
1	H	96	LEU	3.3
1	D	225	ALA	3.3
1	H	64	ALA	3.2
1	D	371	ASP	3.0
1	D	224	GLU	3.0
1	D	226	MET	3.0
1	E	30	GLY	2.9
1	H	81	GLU	2.5
1	D	116	LYS	2.5
1	H	1	MET	2.5
1	H	268	PRO	2.4
1	E	1	MET	2.4
1	D	230	GLU	2.4
1	E	245	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	71	VAL	2.2
1	H	78	MET	2.2
1	H	368	VAL	2.2
1	D	81	GLU	2.2
1	H	267	ILE	2.2
1	G	220	THR	2.1
1	D	353	THR	2.1
1	H	349	LYS	2.0
1	A	243	PHE	2.0
1	A	222	ASP	2.0
1	E	348	ASP	2.0

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

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

6.3 Carbohydrates (i)

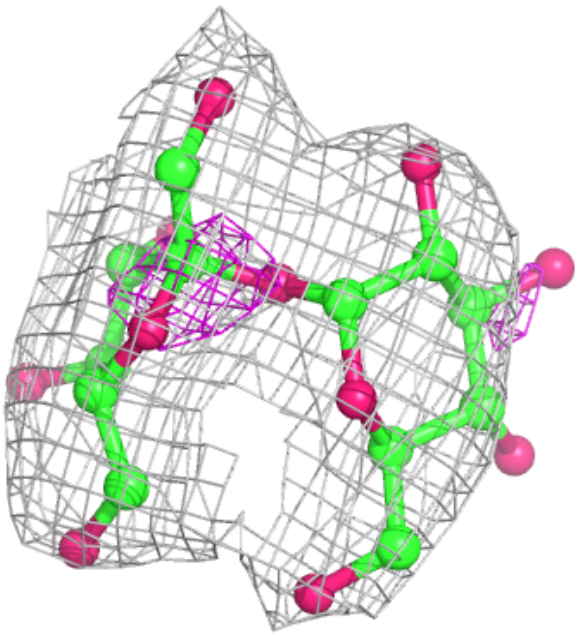
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

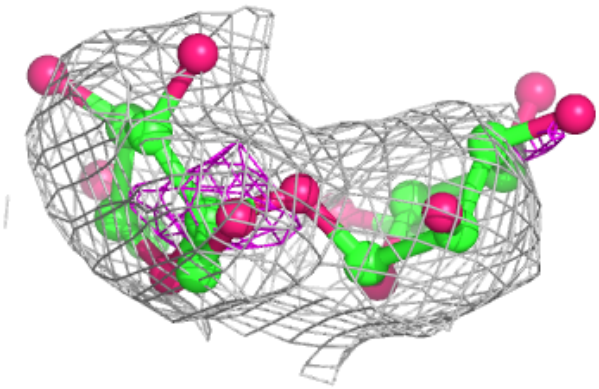
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FRU	K	2	12/12	0.71	0.32	84,88,89,89	0
3	GLC	N	1	11/12	0.71	0.47	97,99,99,99	0
3	FRU	N	2	12/12	0.79	0.36	98,99,99,99	0
3	GLC	O	1	11/12	0.83	0.36	82,83,83,84	0
3	FRU	L	2	12/12	0.85	0.26	81,82,83,83	0
3	FRU	M	2	12/12	0.87	0.27	70,74,75,76	0
3	GLC	J	1	11/12	0.88	0.23	76,77,79,79	0
3	GLC	M	1	11/12	0.88	0.21	76,76,77,77	0
3	GLC	K	1	11/12	0.89	0.26	86,88,88,88	0
3	FRU	O	2	12/12	0.89	0.40	84,85,85,87	0
3	GLC	L	1	11/12	0.90	0.29	79,82,82,83	0
3	FRU	J	2	12/12	0.90	0.20	70,73,75,76	0

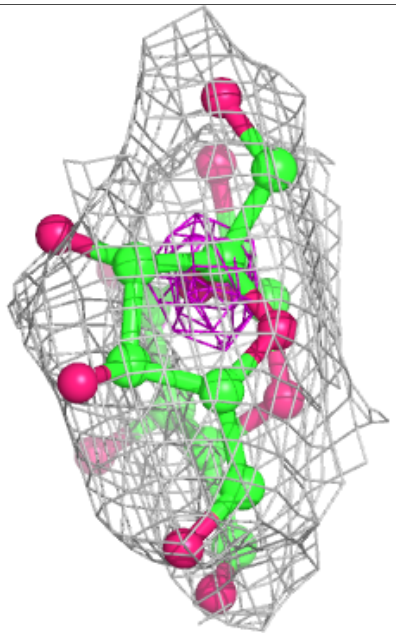
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain J:

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

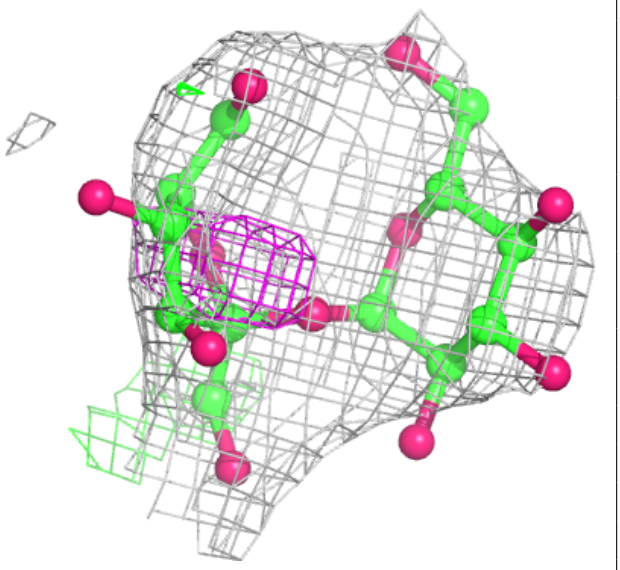


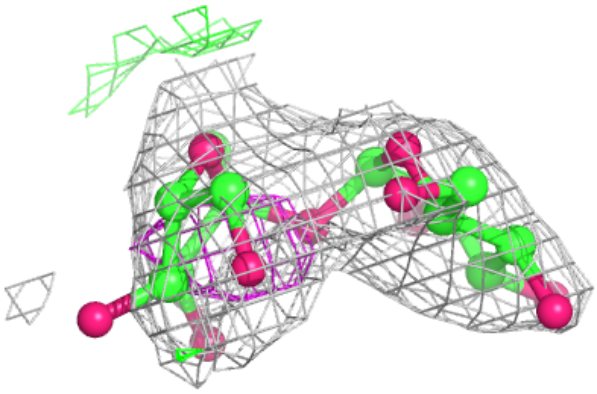


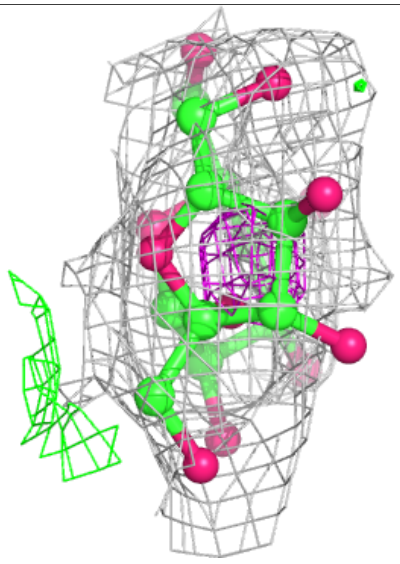


Electron density around Chain K:

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

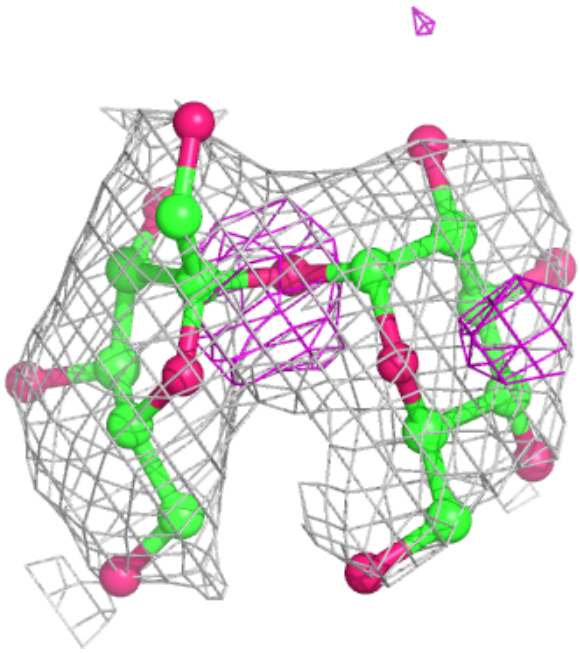


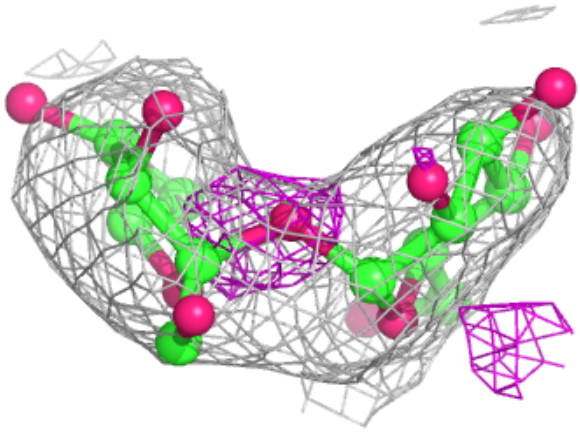


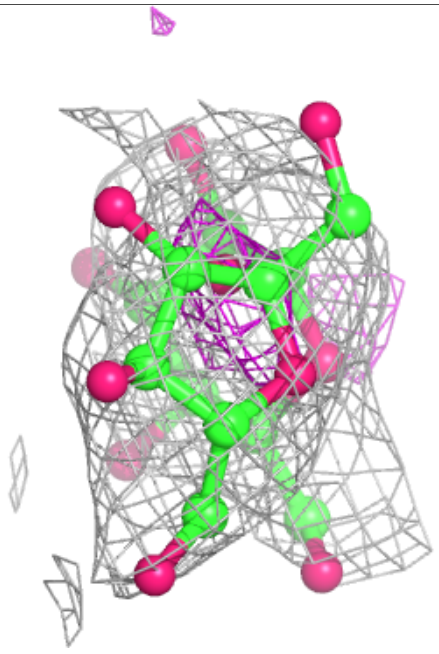


Electron density around Chain L:

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

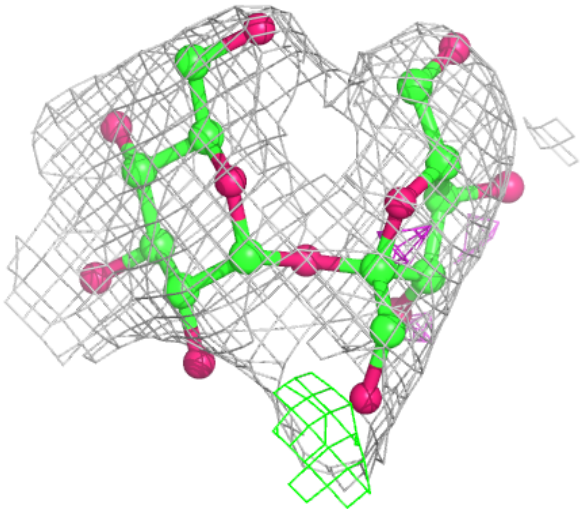


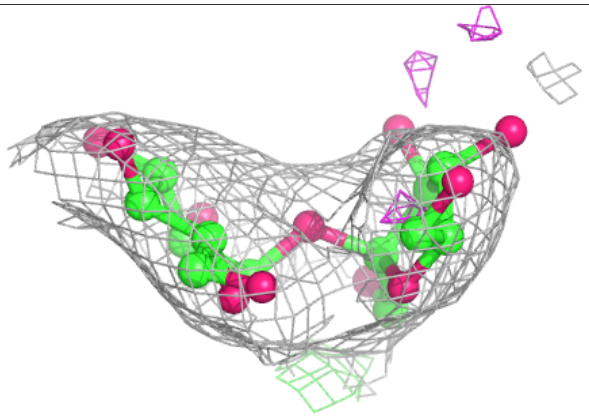


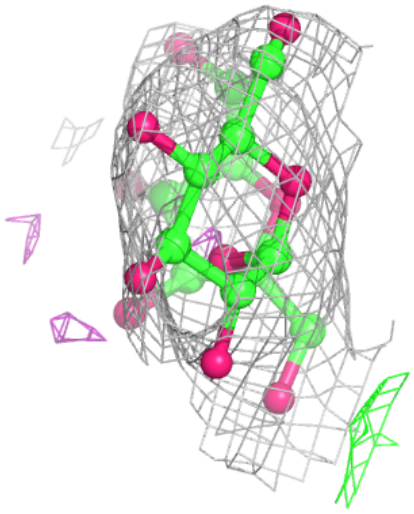


Electron density around Chain M:

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

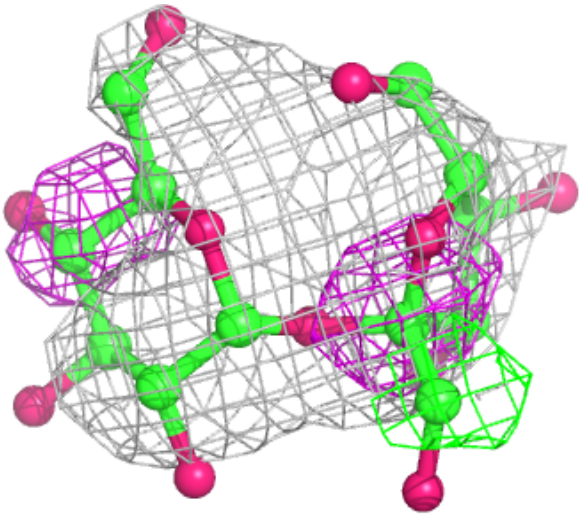


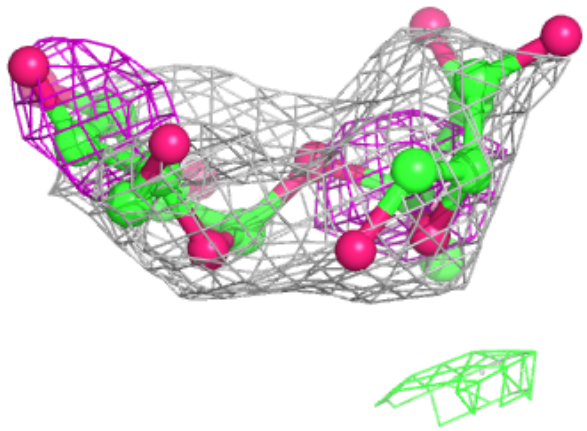


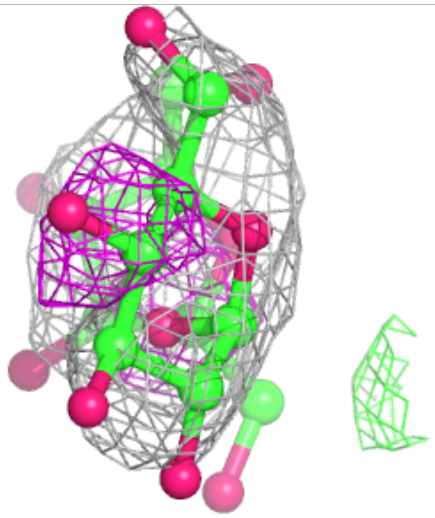


Electron density around Chain N:

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

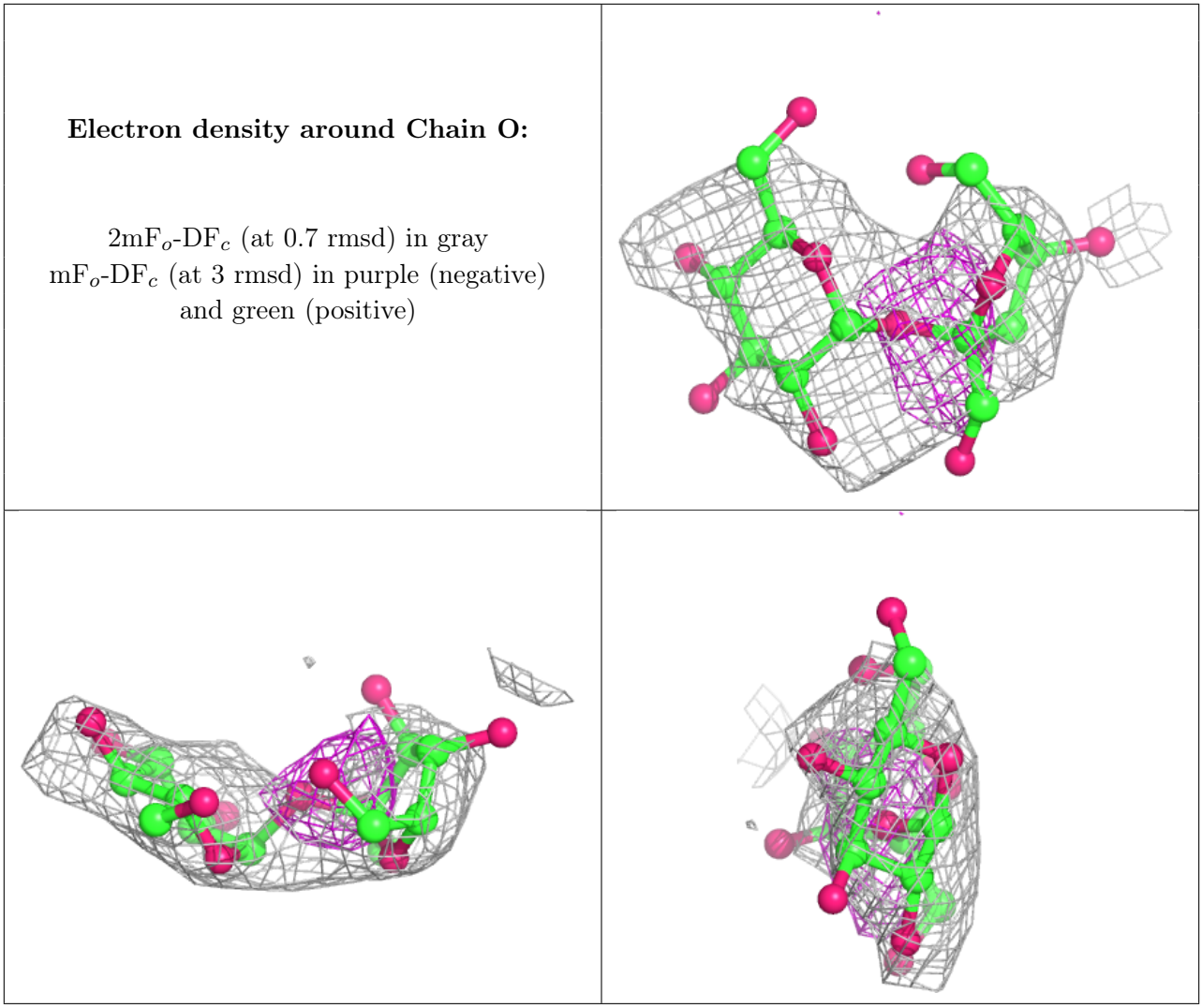






Electron density around Chain O:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAD	B	400	44/44	0.75	0.36	104,104,105,105	0
4	NAD	H	400	44/44	0.85	0.28	88,90,99,101	0
5	NA	A	601	1/1	0.87	0.24	50,50,50,50	0
4	NAD	G	400	44/44	0.90	0.24	65,72,87,87	0
4	NAD	A	400	44/44	0.91	0.21	65,71,75,75	0
5	NA	D	602	1/1	0.92	0.18	69,69,69,69	0
6	NDP	I	500	48/48	0.92	0.17	56,58,64,64	0
4	NAD	D	400	44/44	0.93	0.20	54,60,64,65	0

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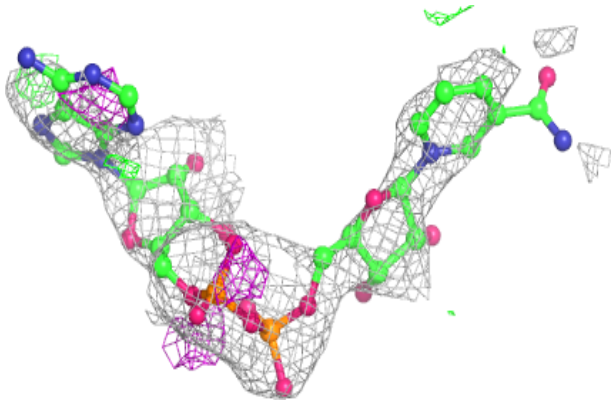
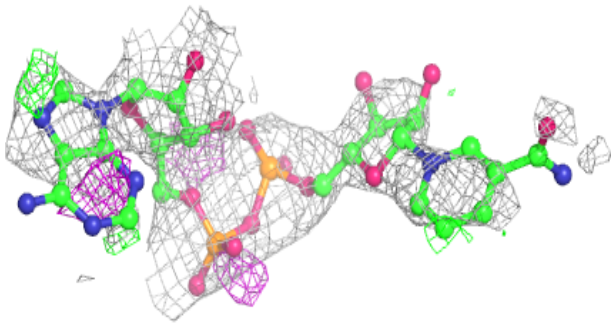
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NDP	F	500	48/48	0.94	0.18	48,52,56,58	0
5	NA	G	603	1/1	0.95	0.10	48,48,48,48	0
6	NDP	C	500	48/48	0.95	0.17	38,40,44,46	0

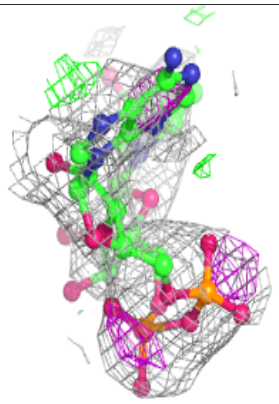
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 400:

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

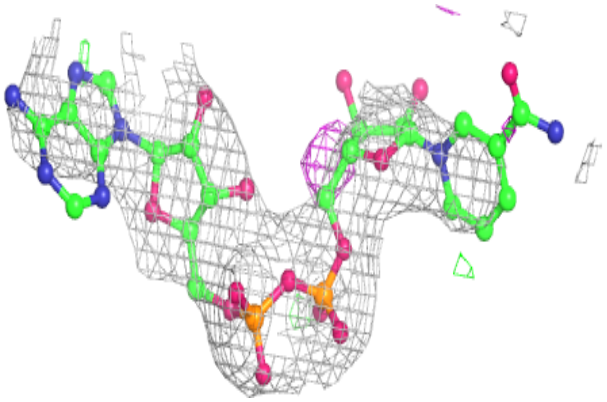


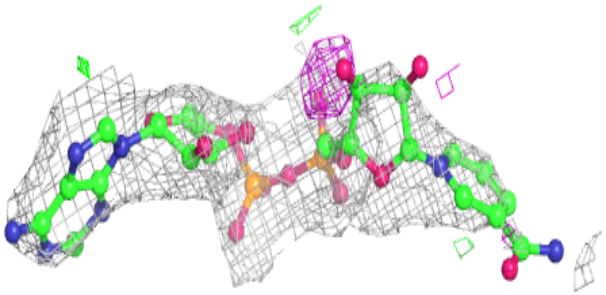


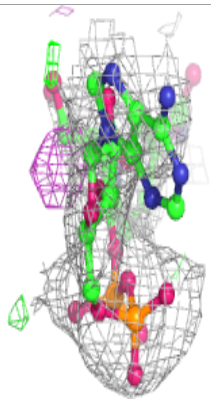


Electron density around NAD H 400:

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

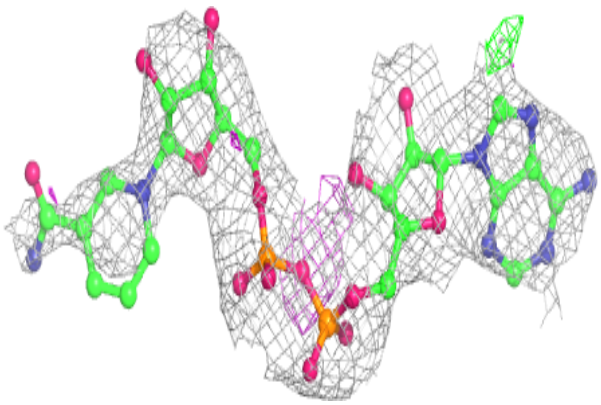


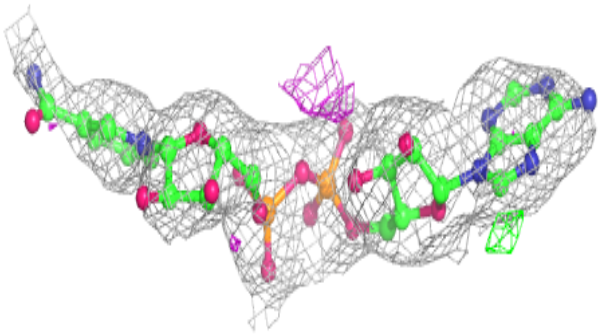


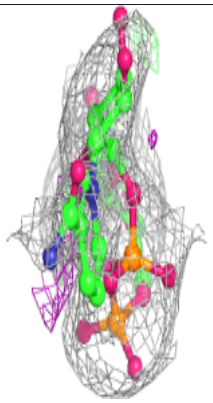


Electron density around NAD G 400:

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

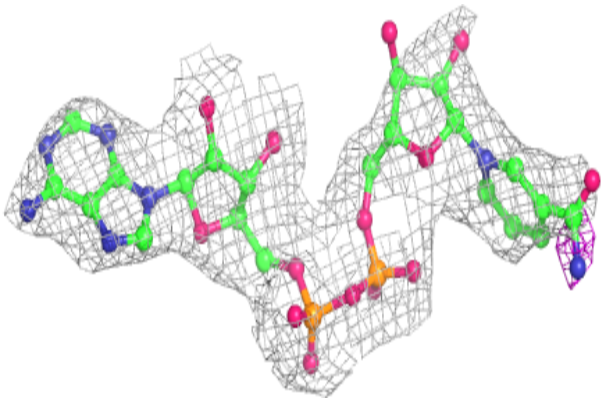


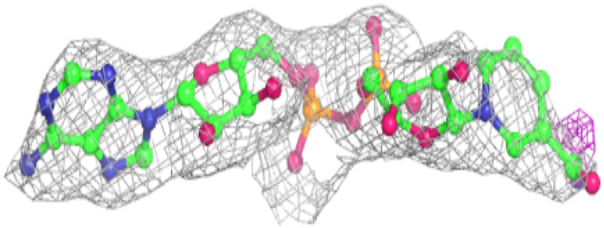


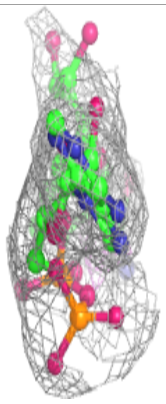


Electron density around NAD A 400:

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

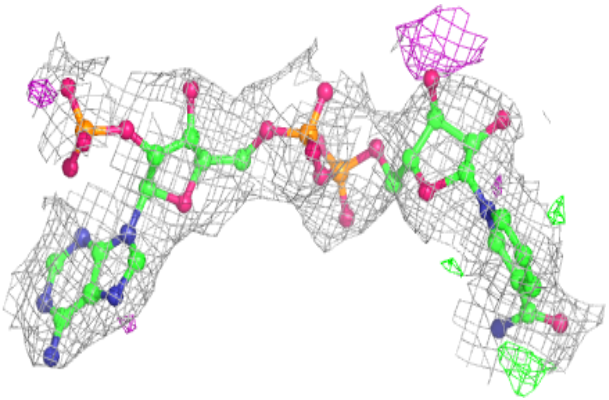


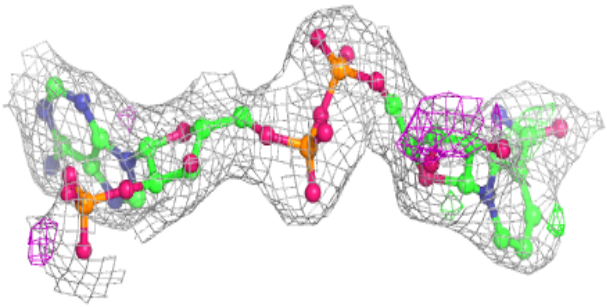


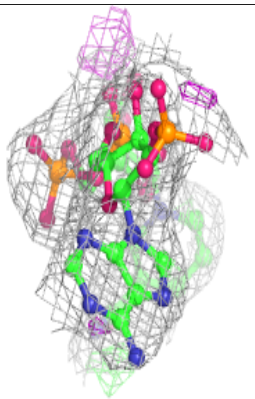


Electron density around NDP I 500:

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

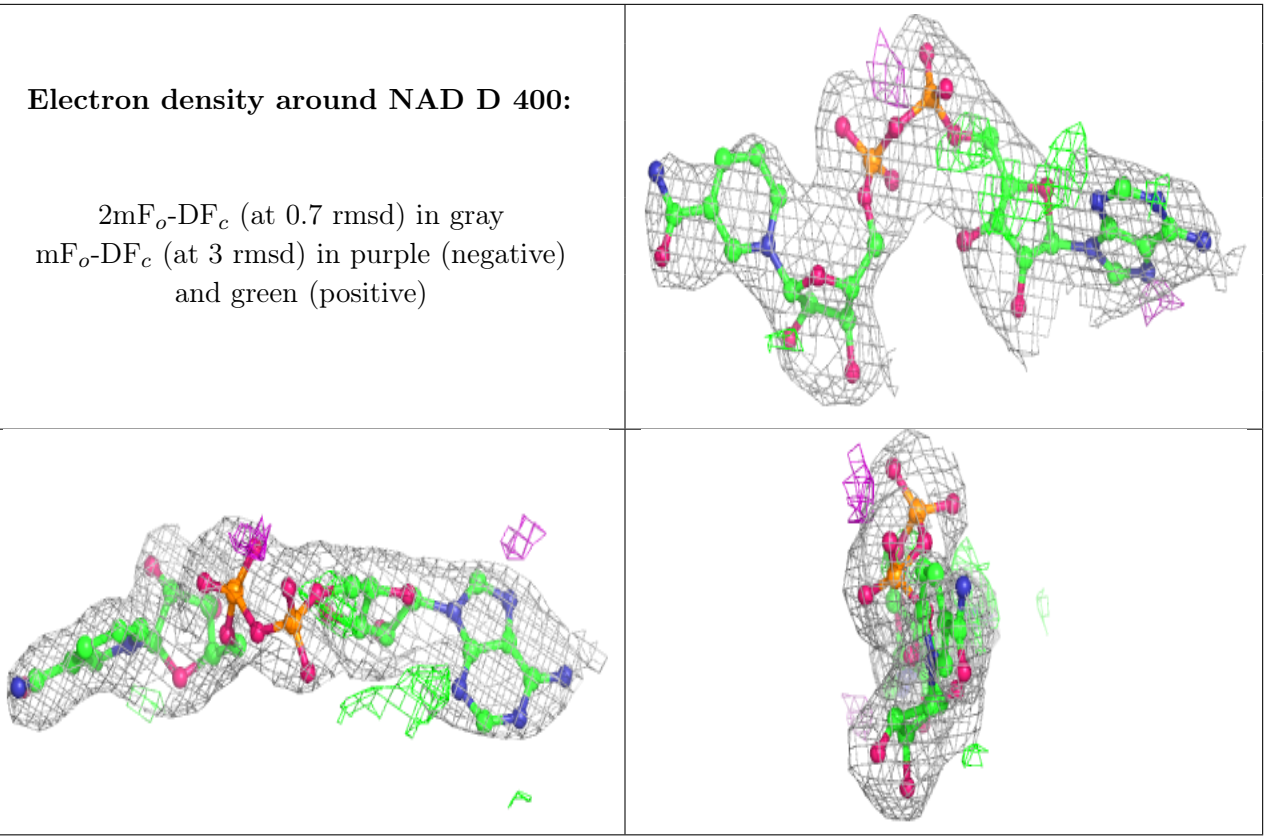






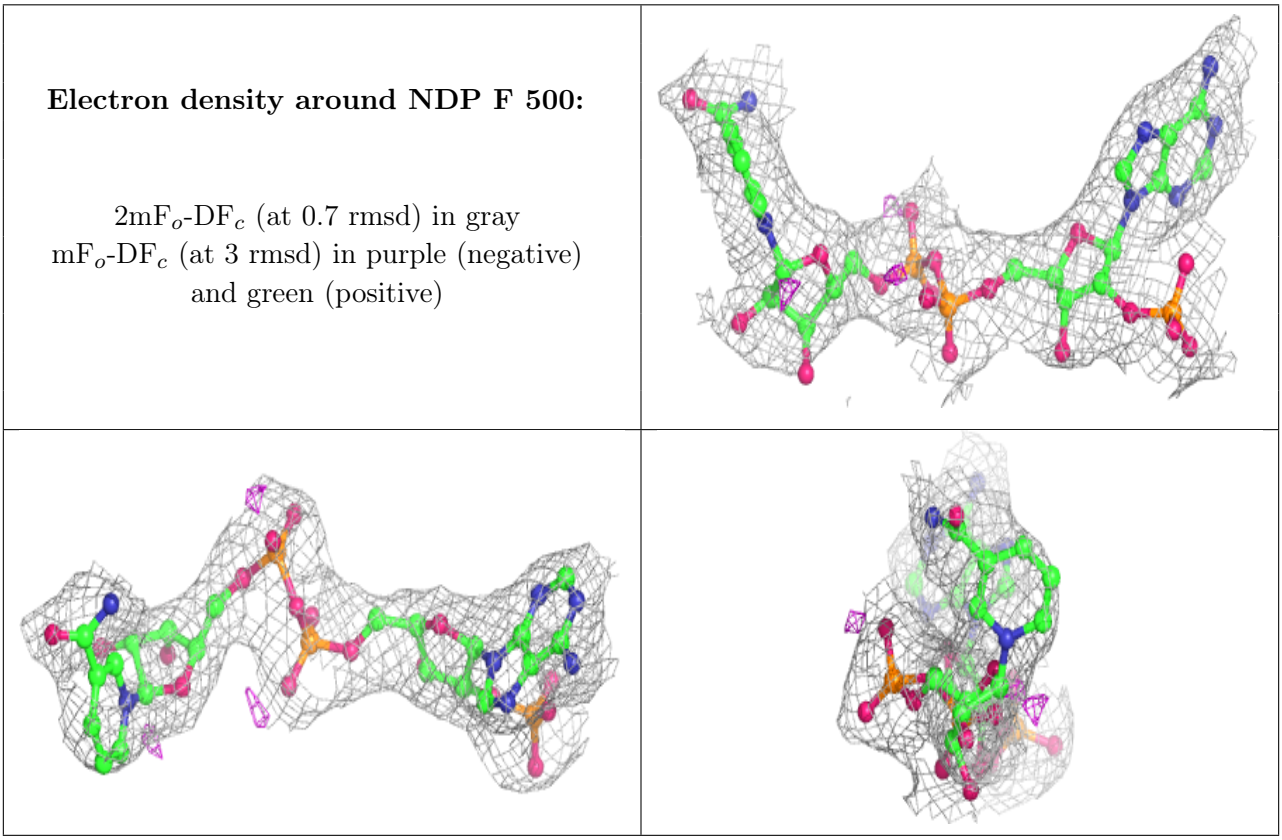
Electron density around NAD D 400:

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



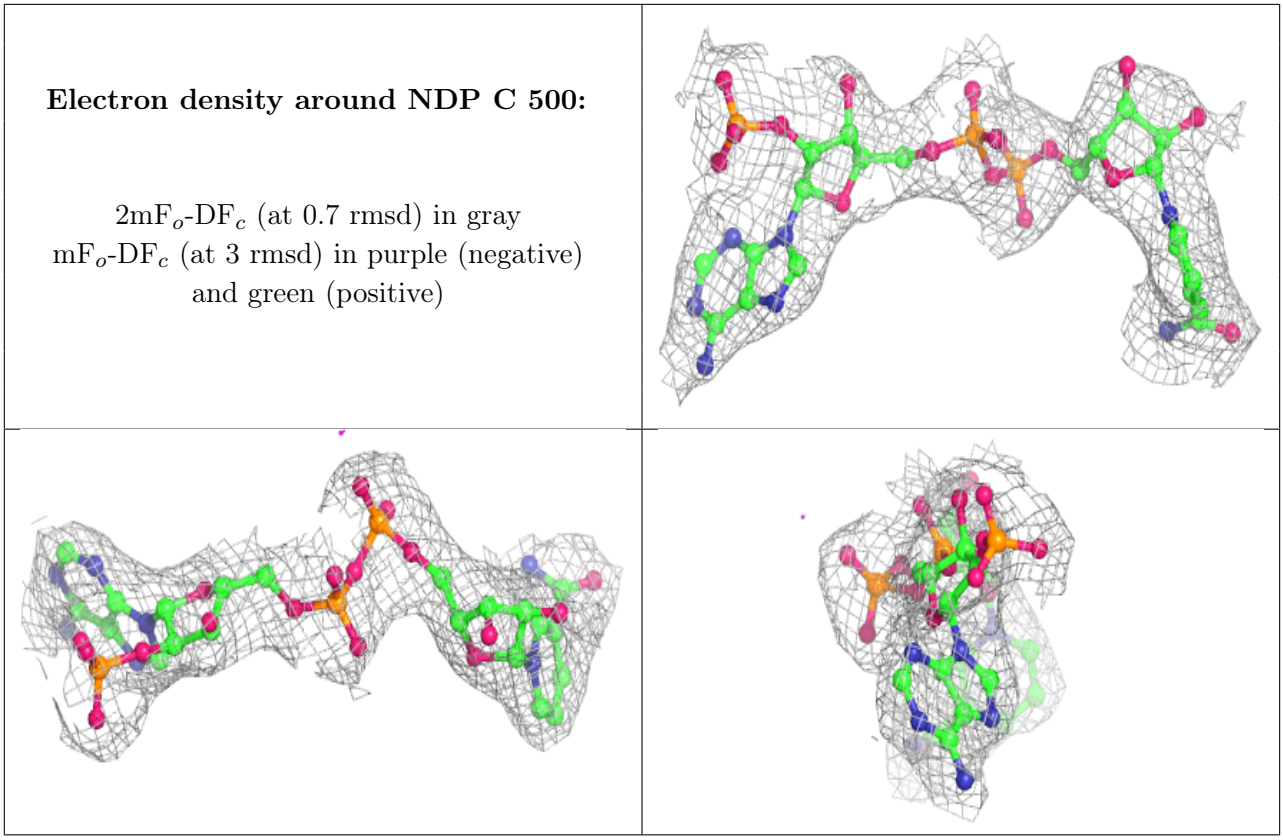
Electron density around NDP F 500:

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



Electron density around NDP C 500:

$2mF_o$-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.