



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 12:16 PM UTC

PDB ID : 1XLT / pdb_00001xlt
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:

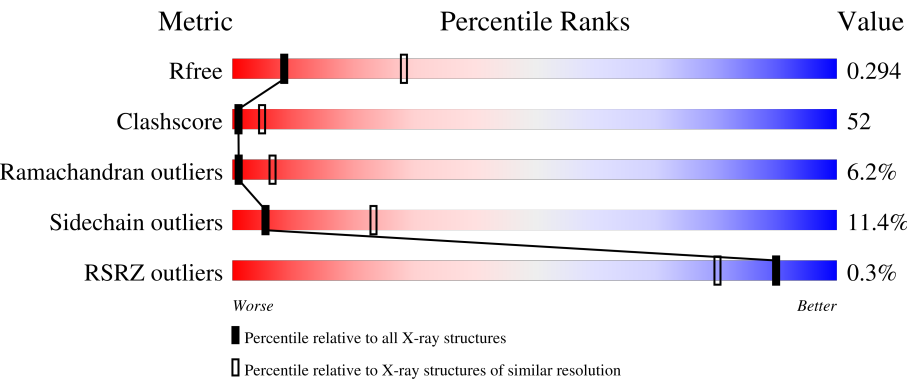
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	384	34%48%12%• 5%
1	B	384	34%46%11%• 7%
1	D	384	% 26%53%16%• •
1	E	384	29%51%11%• 7%
1	G	384	32%51%10%• 5%

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Mol	Chain	Length	Quality of chain
1	H	384	% 24% 49% 18% 7%
2	C	174	39% 50% 10%
2	F	174	40% 52% 6%
2	I	174	30% 55% 13%
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%

2 Entry composition

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:

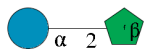
Chain	Residue	Modelled	Actual	Comment	Reference
C	291	ARG	-	cloning artifact	UNP Q59765
C	292	HIS	-	cloning artifact	UNP Q59765
C	293	MET	-	cloning artifact	UNP Q59765
F	291	ARG	-	cloning artifact	UNP Q59765
F	292	HIS	-	cloning artifact	UNP Q59765
F	293	MET	-	cloning artifact	UNP Q59765

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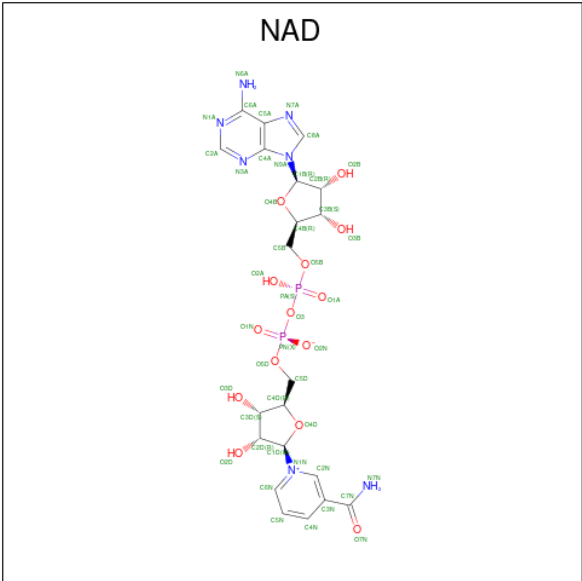
Chain	Residue	Modelled	Actual	Comment	Reference
I	291	ARG	-	cloning artifact	UNP Q59765
I	292	HIS	-	cloning artifact	UNP Q59765
I	293	MET	-	cloning artifact	UNP Q59765

- 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	0	0	0
			23	12	11			
3	K	2	Total	C	O	0	0	0
			23	12	11			
3	L	2	Total	C	O	0	0	0
			23	12	11			
3	M	2	Total	C	O	0	0	0
			23	12	11			
3	N	2	Total	C	O	0	0	0
			23	12	11			
3	O	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

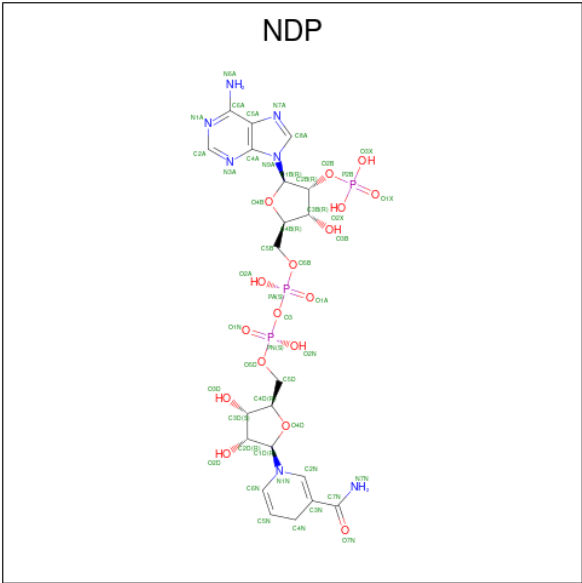


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is SODIUM ION (CCD ID: 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 (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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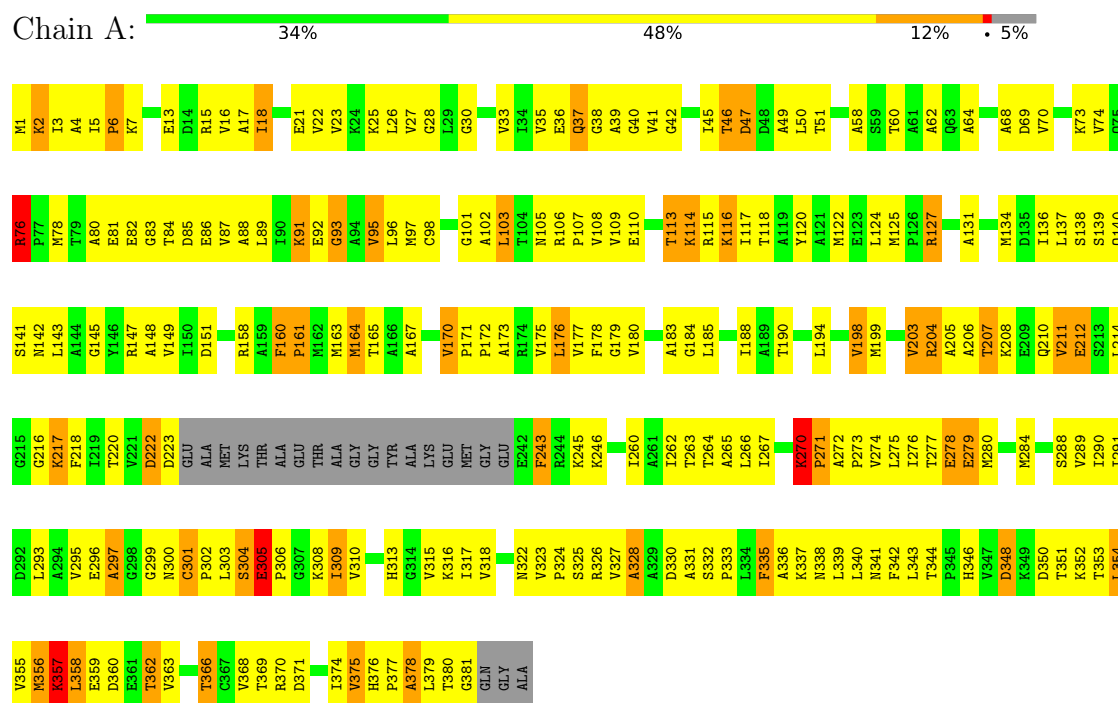
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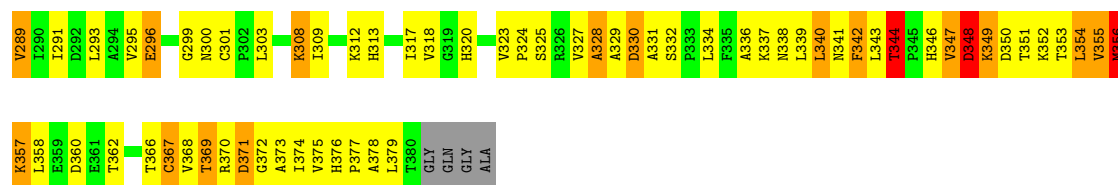
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
6	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

3 Residue-property plots

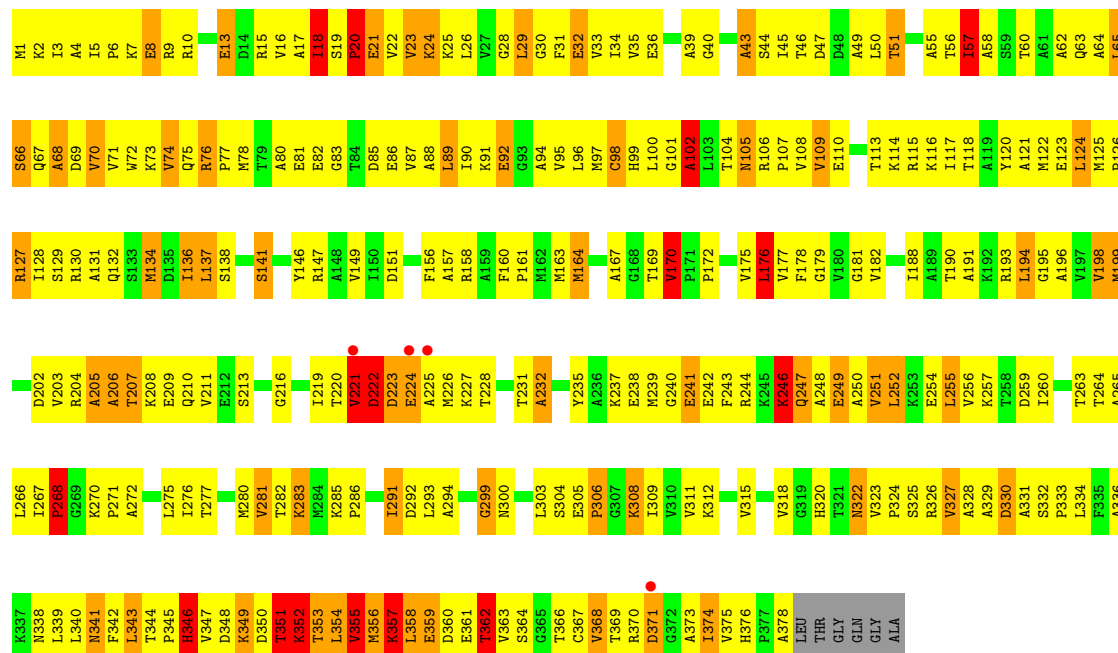
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

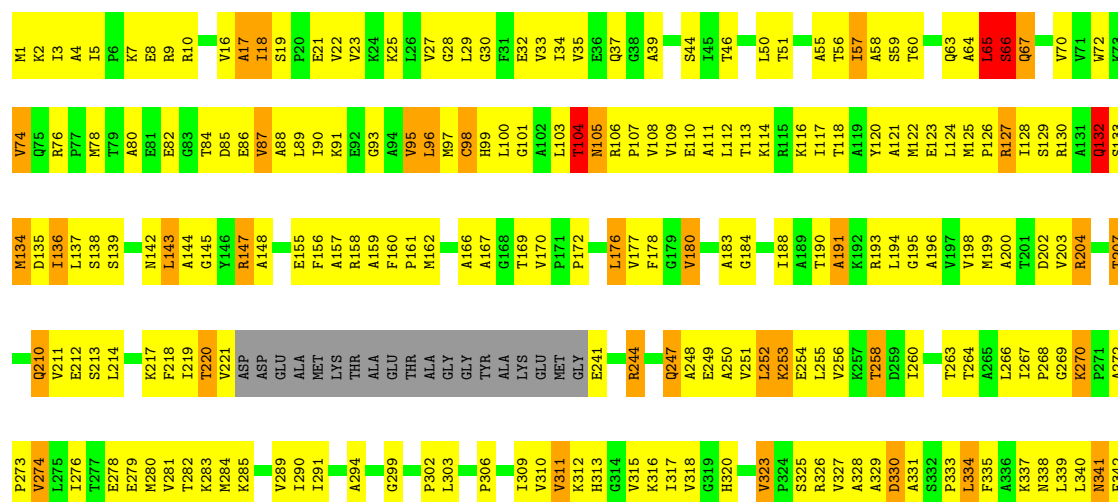


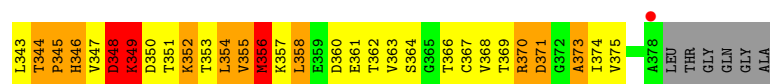


• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



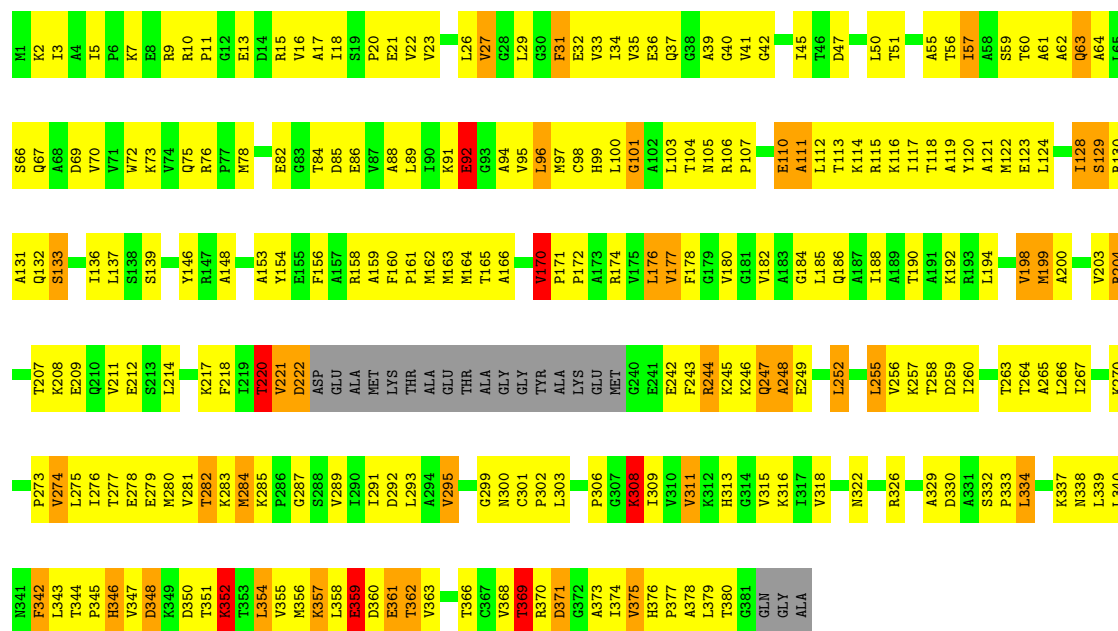
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1





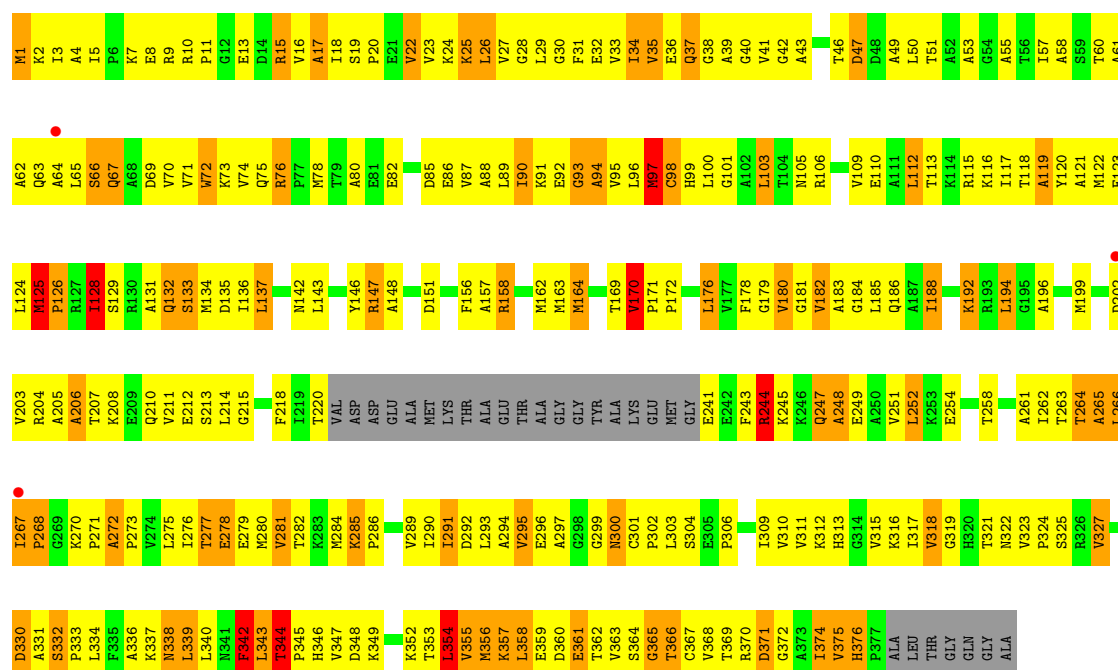
- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

Chain G: 32% 51% 10% 5%

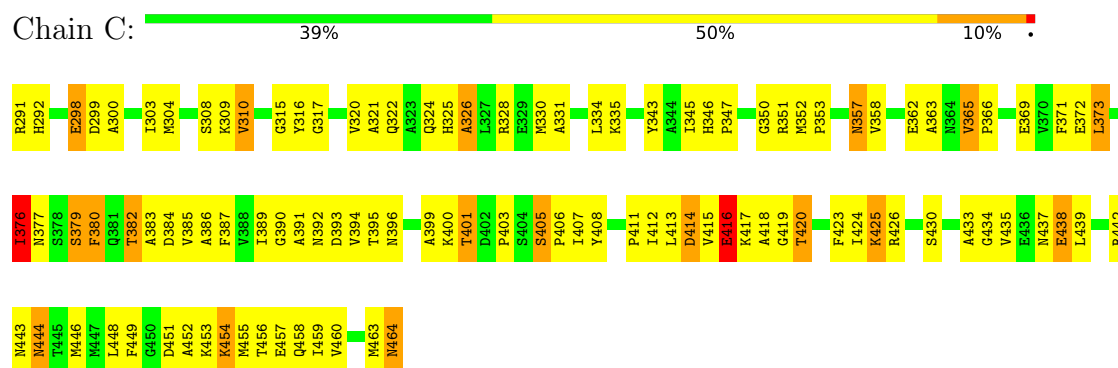


- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

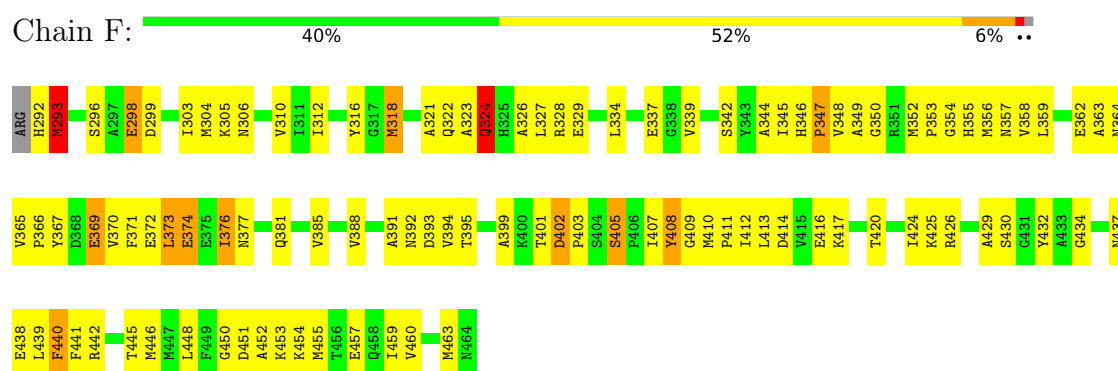
Chain H: 24% 49% 18% 7%



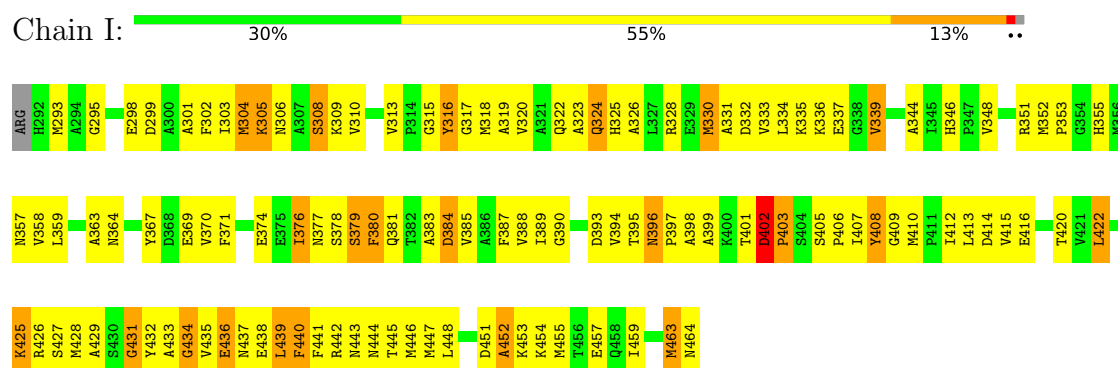
- Molecule 2: NAD(P) transhydrogenase subunit beta



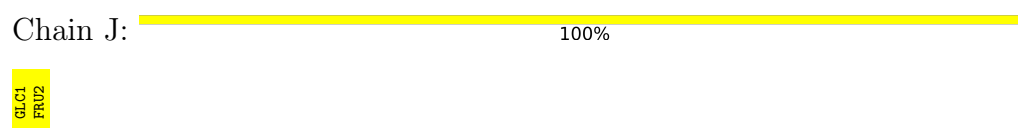
- Molecule 2: NAD(P) transhydrogenase subunit beta



- Molecule 2: NAD(P) transhydrogenase subunit beta



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



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





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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  50% 50%



4 Data and refinement statistics

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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.68-3.10) 96.5 (43.68-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.310 0.227 , 0.294	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)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, FRU, GLC, NA, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	1/2705 (0.0%)	1.21	36/3668 (1.0%)
1	B	0.65	0/2678	1.14	16/3631 (0.4%)
1	D	0.76	0/2816	1.49	56/3816 (1.5%)
1	E	0.69	2/2679 (0.1%)	1.29	33/3632 (0.9%)
1	G	0.62	0/2710	1.21	33/3674 (0.9%)
1	H	0.74	2/2667 (0.1%)	1.47	64/3615 (1.8%)
2	C	0.61	0/1342	1.11	12/1813 (0.7%)
2	F	0.56	0/1331	1.01	5/1799 (0.3%)
2	I	0.65	0/1331	1.25	13/1799 (0.7%)
All	All	0.68	5/20259 (0.0%)	1.28	268/27447 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	ARG	N-CA	-13.58	1.29	1.46
1	E	349	LYS	C-O	8.43	1.35	1.24
1	E	348	ASP	C-N	7.45	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	343	LEU	C-N	-6.96	1.19	1.33
1	H	125	MET	C-O	-5.09	1.17	1.24

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	375	VAL	N-CA-C	24.60	132.97	111.81
1	E	348	ASP	CA-C-N	-13.51	101.53	122.60
1	E	348	ASP	C-N-CA	-13.51	101.53	122.60
1	D	346	HIS	CA-CB-CG	10.73	124.53	113.80
1	D	221	VAL	O-C-N	10.25	136.49	122.97
1	H	267	ILE	CA-C-N	10.08	131.40	120.11
1	H	267	ILE	C-N-CA	10.08	131.40	120.11
2	I	402	ASP	CA-C-O	9.49	133.16	120.16
1	D	374	ILE	CA-C-O	9.35	132.47	120.78
1	D	67	GLN	O-C-N	-9.03	110.58	122.59
1	H	371	ASP	CA-CB-CG	9.02	121.62	112.60
1	H	170	VAL	CA-C-N	8.94	126.19	119.66
1	H	170	VAL	C-N-CA	8.94	126.19	119.66
1	H	342	PHE	CA-CB-CG	8.79	122.58	113.80
1	G	357	LYS	CA-C-N	8.61	137.99	121.54
1	G	357	LYS	C-N-CA	8.61	137.99	121.54
2	I	403	PRO	CA-N-CD	-8.60	99.97	112.00
1	D	221	VAL	N-CA-CB	8.49	121.14	111.21
1	H	285	LYS	CA-C-N	8.37	128.38	119.76
1	H	285	LYS	C-N-CA	8.37	128.38	119.76
1	G	357	LYS	O-C-N	-8.20	111.68	122.59
1	A	198	VAL	N-CA-C	8.20	120.39	108.58
1	G	350	ASP	CA-CB-CG	8.05	120.65	112.60
1	E	349	LYS	CA-C-O	-8.04	110.10	119.59
1	H	126	PRO	CA-N-CD	-8.02	100.77	112.00
1	D	362	THR	N-CA-C	-7.99	103.43	113.02
1	B	267	ILE	CA-C-N	7.92	129.74	119.84
1	B	267	ILE	C-N-CA	7.92	129.74	119.84
1	D	371	ASP	CA-CB-CG	7.84	120.44	112.60
1	H	345	PRO	CA-N-CD	-7.74	101.17	112.00
1	A	243	PHE	N-CA-C	-7.62	103.44	112.89
2	I	380	PHE	N-CA-C	-7.61	102.96	111.71
1	D	57	ILE	CA-C-N	7.56	134.46	122.21
1	D	57	ILE	C-N-CA	7.56	134.46	122.21
1	D	170	VAL	CA-C-N	7.53	125.08	119.66
1	D	170	VAL	C-N-CA	7.53	125.08	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	317	ILE	O-C-N	-7.52	113.17	122.57
1	G	352	LYS	CA-C-O	7.51	130.82	122.03
1	D	57	ILE	CA-C-O	-7.51	114.07	121.58
1	H	125	MET	O-C-N	7.46	129.90	121.32
1	E	220	THR	N-CA-C	-7.46	103.23	111.36
1	H	365	GLY	CA-C-N	7.36	135.60	121.54
1	H	365	GLY	C-N-CA	7.36	135.60	121.54
1	A	356	MET	CA-C-N	7.31	135.51	121.54
1	A	356	MET	C-N-CA	7.31	135.51	121.54
1	D	251	VAL	N-CA-C	-7.31	105.88	112.90
1	D	132	GLN	N-CA-C	-7.29	104.53	113.50
1	H	125	MET	CA-C-N	-7.24	110.79	119.84
1	H	125	MET	C-N-CA	-7.24	110.79	119.84
1	G	112	LEU	N-CA-C	-7.19	104.13	113.12
1	H	344	THR	N-CA-C	7.17	125.67	109.81
1	G	242	GLU	N-CA-C	-7.15	103.82	112.54
2	I	369	GLU	N-CA-C	-7.08	104.25	113.17
2	C	326	ALA	N-CA-C	-7.08	103.50	111.07
1	E	350	ASP	CA-C-N	7.08	132.02	120.63
1	E	350	ASP	C-N-CA	7.08	132.02	120.63
1	A	47	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	220	THR	N-CA-C	7.07	120.12	109.95
1	E	101	GLY	N-CA-C	-7.06	101.06	113.76
1	E	66	SER	CA-C-N	7.01	134.02	122.73
1	E	66	SER	C-N-CA	7.01	134.02	122.73
1	G	282	THR	N-CA-C	-7.00	105.28	114.31
1	G	308	LYS	N-CA-C	7.00	117.27	108.45
1	E	99	HIS	N-CA-C	-6.99	98.33	109.59
1	B	57	ILE	N-CA-C	6.98	117.89	108.11
1	H	268	PRO	N-CA-C	6.98	121.31	111.33
1	H	133	SER	O-C-N	-6.96	113.33	122.59
1	A	309	ILE	N-CA-C	-6.95	98.15	109.12
2	I	304	MET	N-CA-C	6.94	121.80	113.12
2	I	396	ASN	CA-C-N	6.91	126.51	119.19
2	I	396	ASN	C-N-CA	6.91	126.51	119.19
2	C	405	SER	CA-C-N	6.86	128.41	119.84
2	C	405	SER	C-N-CA	6.86	128.41	119.84
1	A	357	LYS	CA-C-N	6.83	134.59	121.54
1	A	357	LYS	C-N-CA	6.83	134.59	121.54
1	D	359	GLU	N-CA-C	-6.77	103.98	111.36
1	H	133	SER	CA-C-O	6.75	130.16	120.51
1	B	323	VAL	CA-C-N	-6.72	111.88	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	VAL	C-N-CA	-6.72	111.88	119.28
1	A	350	ASP	N-CA-C	6.71	120.69	112.23
1	E	352	LYS	CA-C-O	6.67	129.58	121.84
1	D	346	HIS	ND1-CE1-NE2	-6.67	101.73	108.40
1	H	171	PRO	N-CA-C	6.63	116.84	110.47
1	D	220	THR	O-C-N	-6.62	113.78	122.59
1	D	283	LYS	N-CA-C	-6.60	104.95	114.12
1	D	206	ALA	N-CA-C	-6.59	104.24	113.20
1	H	300	ASN	N-CA-C	-6.57	105.02	113.16
1	G	101	GLY	N-CA-C	-6.56	103.90	113.48
1	D	350	ASP	CA-C-N	6.53	134.02	121.54
1	D	350	ASP	C-N-CA	6.53	134.02	121.54
1	A	171	PRO	CA-C-N	6.51	126.47	120.03
1	A	171	PRO	C-N-CA	6.51	126.47	120.03
1	D	222	ASP	CA-C-N	6.47	133.16	122.62
1	D	222	ASP	C-N-CA	6.47	133.16	122.62
1	H	94	ALA	N-CA-C	6.43	118.32	110.41
1	D	221	VAL	CA-C-N	6.38	133.73	121.54
1	D	221	VAL	C-N-CA	6.38	133.73	121.54
1	H	182	VAL	N-CA-C	-6.38	104.94	110.74
1	G	133	SER	CA-C-O	6.37	127.14	119.43
1	E	65	LEU	CA-C-N	6.34	133.64	121.54
1	E	65	LEU	C-N-CA	6.34	133.64	121.54
1	A	306	PRO	N-CA-C	6.32	120.35	110.80
2	C	357	ASN	N-CA-C	6.29	117.83	110.97
2	C	401	THR	N-CA-C	6.28	114.78	108.75
1	B	367	CYS	N-CA-C	6.26	119.91	110.64
2	I	305	LYS	N-CA-C	-6.25	105.75	113.19
2	C	365	VAL	CA-C-N	6.24	127.64	119.84
2	C	365	VAL	C-N-CA	6.24	127.64	119.84
1	G	350	ASP	CA-C-N	6.22	132.56	120.99
1	G	350	ASP	C-N-CA	6.22	132.56	120.99
1	D	105	ASN	CA-CB-CG	6.21	118.81	112.60
1	A	305	GLU	CA-C-N	6.21	126.42	119.90
1	A	305	GLU	C-N-CA	6.21	126.42	119.90
2	C	376	ILE	N-CA-C	6.21	117.22	111.45
1	A	335	PHE	N-CA-C	-6.20	104.60	111.36
1	H	272	ALA	CA-C-N	6.19	127.58	119.84
1	H	272	ALA	C-N-CA	6.19	127.58	119.84
1	H	376	HIS	O-C-N	-6.19	114.60	121.53
1	D	272	ALA	CA-C-N	6.17	126.38	119.90
1	D	272	ALA	C-N-CA	6.17	126.38	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	LYS	N-CA-C	-6.17	104.62	111.71
1	D	116	LYS	CA-C-O	6.13	128.57	121.28
1	E	354	LEU	O-C-N	6.12	130.23	123.01
1	A	173	ALA	N-CA-C	-6.11	102.64	110.53
1	A	206	ALA	N-CA-C	-6.09	105.70	113.01
1	D	223	ASP	N-CA-C	6.08	118.75	110.06
1	E	349	LYS	CB-CA-C	6.07	120.98	110.72
1	D	352	LYS	CA-C-N	6.04	133.08	121.54
1	D	352	LYS	C-N-CA	6.04	133.08	121.54
1	H	206	ALA	N-CA-C	-6.03	105.41	112.89
1	G	287	GLY	N-CA-C	-6.03	106.32	115.00
1	H	343	LEU	CA-C-N	6.03	136.51	121.80
1	H	343	LEU	C-N-CA	6.03	136.51	121.80
1	H	366	THR	CA-C-N	5.97	129.24	120.82
1	H	366	THR	C-N-CA	5.97	129.24	120.82
1	A	101	GLY	N-CA-C	-5.96	103.03	113.76
1	A	214	LEU	N-CA-C	-5.91	106.23	113.50
1	H	344	THR	CA-C-N	-5.90	113.68	119.64
1	H	344	THR	C-N-CA	-5.90	113.68	119.64
1	D	89	LEU	N-CA-C	-5.90	104.93	111.36
1	E	285	LYS	CA-C-N	5.88	125.90	119.90
1	E	285	LYS	C-N-CA	5.88	125.90	119.90
1	D	116	LYS	CA-C-N	-5.87	115.52	123.10
1	D	116	LYS	C-N-CA	-5.87	115.52	123.10
1	H	128	ILE	CA-C-N	5.87	133.03	122.46
1	H	128	ILE	C-N-CA	5.87	133.03	122.46
1	H	272	ALA	N-CA-C	5.86	118.22	110.36
1	B	344	THR	N-CA-C	5.86	122.75	109.81
1	H	266	LEU	N-CA-C	5.85	117.68	108.96
1	H	264	THR	N-CA-C	-5.83	106.08	113.43
1	H	80	ALA	N-CA-C	-5.83	105.42	112.54
1	H	17	ALA	CA-C-O	5.82	126.25	120.32
1	E	166	ALA	N-CA-C	-5.81	105.45	112.54
1	H	93	GLY	N-CA-C	-5.80	106.99	115.63
1	B	61	ALA	N-CA-C	-5.79	104.32	111.33
1	G	359	GLU	N-CA-C	-5.78	106.20	113.20
2	I	330	MET	N-CA-C	-5.78	104.89	111.07
1	G	354	LEU	CA-C-N	-5.78	114.77	122.98
1	G	354	LEU	C-N-CA	-5.78	114.77	122.98
1	A	297	ALA	N-CA-C	-5.77	104.47	112.03
1	G	170	VAL	CA-C-N	5.77	123.81	119.66
1	G	170	VAL	C-N-CA	5.77	123.81	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	341	ASN	O-C-N	-5.76	114.93	122.59
1	G	246	LYS	N-CA-C	-5.75	105.84	112.92
2	F	362	GLU	N-CA-C	-5.75	104.93	111.14
1	B	356	MET	O-C-N	-5.75	114.48	122.41
1	B	308	LYS	N-CA-C	5.72	117.92	109.69
2	I	403	PRO	N-CA-CB	5.70	109.23	103.25
1	H	125	MET	C-N-CD	5.68	148.30	125.00
1	H	119	ALA	N-CA-C	5.68	119.50	109.96
1	E	67	GLN	CA-C-O	5.66	126.52	119.78
1	H	301	CYS	CA-C-N	5.63	125.73	119.32
1	H	301	CYS	C-N-CA	5.63	125.73	119.32
1	B	330	ASP	CA-CB-CG	5.62	118.22	112.60
1	E	341	ASN	N-CA-C	-5.61	105.08	111.14
1	E	311	VAL	N-CA-C	5.59	116.56	106.61
1	G	220	THR	N-CA-C	5.58	117.90	110.53
1	E	373	ALA	N-CA-C	5.58	115.91	108.38
1	G	133	SER	O-C-N	-5.57	115.20	122.39
2	F	426	ARG	N-CA-C	5.56	117.34	111.28
1	G	171	PRO	N-CA-C	5.53	116.49	110.58
1	D	226	MET	N-CA-C	-5.51	106.87	113.21
1	B	131	ALA	N-CA-C	5.50	119.25	112.54
1	H	188	ILE	N-CA-C	-5.50	105.01	111.00
1	A	301	CYS	CA-C-N	5.50	125.84	119.47
1	A	301	CYS	C-N-CA	5.50	125.84	119.47
1	G	131	ALA	CA-C-N	5.49	132.02	121.54
1	G	131	ALA	C-N-CA	5.49	132.02	121.54
1	E	356	MET	O-C-N	-5.49	115.29	122.59
1	D	104	THR	CA-C-O	5.47	125.20	119.51
1	H	366	THR	CA-CB-CG2	5.46	119.79	110.50
1	A	76	ARG	CA-C-N	5.45	126.65	119.84
1	A	76	ARG	C-N-CA	5.45	126.65	119.84
1	D	375	VAL	N-CA-C	-5.44	104.29	111.09
1	H	374	ILE	O-C-N	5.44	128.69	122.93
1	D	308	LYS	N-CA-C	5.44	117.67	109.41
1	H	248	ALA	N-CA-C	-5.43	106.49	113.01
1	D	349	LYS	N-CA-C	-5.42	106.35	113.12
1	D	57	ILE	CA-CB-CG2	5.42	119.71	110.50
1	H	171	PRO	CA-C-N	5.39	125.69	119.92
1	H	171	PRO	C-N-CA	5.39	125.69	119.92
1	A	161	PRO	N-CA-C	5.39	118.77	111.22
1	G	342	PHE	N-CA-C	-5.38	106.56	113.23
1	D	68	ALA	CA-C-N	5.37	131.80	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	68	ALA	C-N-CA	5.37	131.80	121.54
2	I	308	SER	N-CA-C	-5.35	106.69	113.43
1	H	371	ASP	O-C-N	-5.34	115.48	122.59
1	A	27	VAL	N-CA-C	-5.34	105.17	110.62
1	H	97	MET	CA-C-N	5.33	131.72	121.54
1	H	97	MET	C-N-CA	5.33	131.72	121.54
1	D	213	SER	N-CA-C	-5.32	106.74	113.18
1	E	355	VAL	O-C-N	-5.32	115.92	122.57
1	G	355	VAL	O-C-N	-5.29	117.68	123.18
1	G	198	VAL	N-CA-C	5.27	117.45	109.12
1	B	39	ALA	N-CA-C	-5.26	106.90	113.38
1	A	102	ALA	N-CA-C	5.26	116.70	111.07
2	C	400	LYS	CA-C-N	5.25	128.75	123.13
2	C	400	LYS	C-N-CA	5.25	128.75	123.13
2	F	440	PHE	N-CA-C	-5.25	106.94	113.19
1	A	116	LYS	N-CA-C	-5.25	106.83	113.23
1	E	317	ILE	CA-C-O	5.22	127.30	120.78
1	H	126	PRO	N-CD-CG	5.21	111.02	103.20
1	H	343	LEU	CA-C-O	-5.20	113.07	120.51
1	B	287	GLY	N-CA-C	-5.19	108.51	114.69
1	D	246	LYS	CA-C-N	5.19	131.46	121.54
1	D	246	LYS	C-N-CA	5.19	131.46	121.54
1	A	348	ASP	N-CA-C	-5.19	102.70	110.23
2	C	345	ILE	N-CA-C	5.18	115.04	107.37
1	D	357	LYS	N-CA-C	5.18	121.84	110.80
2	F	405	SER	N-CA-C	5.17	116.58	110.07
1	E	323	VAL	CB-CA-C	-5.16	108.88	114.35
1	D	57	ILE	CA-CB-CG1	5.16	119.17	110.40
1	A	270	LYS	N-CA-C	5.15	121.19	109.81
1	D	198	VAL	N-CA-C	5.15	116.66	109.55
2	F	369	GLU	N-CA-C	-5.15	105.88	113.61
1	G	284	MET	N-CA-C	5.15	117.69	109.81
1	D	220	THR	CA-C-N	-5.14	116.32	122.90
1	D	220	THR	C-N-CA	-5.14	116.32	122.90
1	H	47	ASP	N-CA-C	-5.13	105.38	110.97
1	B	115	ARG	N-CA-C	-5.13	106.87	113.02
2	I	436	GLU	N-CA-C	-5.12	102.48	110.42
1	E	248	ALA	N-CA-C	-5.11	106.88	113.01
1	H	332	SER	CA-C-N	-5.11	113.66	119.28
1	H	332	SER	C-N-CA	-5.11	113.66	119.28
1	H	366	THR	N-CA-CB	5.10	119.12	110.49
1	E	66	SER	CA-C-O	-5.10	113.22	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	352	LYS	N-CA-CB	5.10	118.91	111.62
1	H	366	THR	N-CA-C	5.09	121.65	110.80
1	B	245	LYS	N-CA-C	-5.09	105.86	111.71
1	A	279	GLU	N-CA-C	-5.09	105.42	110.97
1	G	267	ILE	CA-C-N	5.08	125.37	119.93
1	G	267	ILE	C-N-CA	5.08	125.37	119.93
1	A	203	VAL	N-CA-C	-5.08	105.90	110.82
2	I	339	VAL	N-CA-C	5.08	119.90	109.34
1	D	331	ALA	N-CA-C	5.07	118.24	111.75
1	D	330	ASP	N-CA-C	-5.07	105.45	111.69
1	E	191	ALA	N-CA-C	-5.07	105.26	111.75
1	E	247	GLN	N-CA-C	-5.06	106.20	112.93
1	E	132	GLN	N-CA-C	5.06	118.22	111.75
1	H	375	VAL	CB-CA-C	-5.05	105.74	111.55
1	G	346	HIS	N-CA-C	-5.04	106.38	112.88
1	A	145	GLY	N-CA-C	-5.03	108.08	114.16
1	D	351	THR	CA-C-O	5.03	127.70	120.51
1	H	126	PRO	N-CA-CB	5.03	108.53	103.25
1	D	43	ALA	N-CA-C	-5.02	107.20	113.72
1	A	160	PHE	N-CA-C	5.01	119.07	112.35
1	E	143	LEU	N-CA-C	-5.01	105.72	111.14
2	C	389	ILE	N-CA-C	5.00	114.78	107.37

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 ⓘ

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	226	0
1	B	2643	0	2784	278	0
1	D	2779	0	2904	392	0
1	E	2644	0	2781	290	0
1	G	2675	0	2809	264	0
1	H	2632	0	2766	425	0
2	C	1318	0	1305	124	0
2	F	1307	0	1292	109	0
2	I	1307	0	1292	137	0
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	5	0
6	F	48	0	26	10	0
6	I	48	0	26	3	0
All	All	20480	0	21066	2159	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 52.

All (2159) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:186:GLN:HA	2:I:352:MET:HE1	1.33	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
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: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:D:97:MET:HB2	1:D:122:MET:HE1	1.42	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:D:163:MET:HE1	1:E:142:ASN:HD21	1.28	0.98
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:E:125:MET:HE1	1:E:342:PHE:HD2	1.29	0.97
1:A:270:LYS:HB2	1:A:271:PRO:CD	1.95	0.96
1:A:163:MET:HE3	1:A:170:VAL:HG11	1.46	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:A:97:MET:HE1	1:A:343:LEU:HD12	1.48	0.95
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:446:MET:HE3	2:F:448:LEU:HD21	1.47	0.94
1:H:131:ALA:HA	1:H:134:MET:HE3	1.47	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
1:B:164:MET:HA	1:B:164:MET:HE3	1.46	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
2:C:464:ASN:C	2:C:464:ASN:HD22	1.77	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
1:D:134:MET:HE2	1:D:341:ASN:O	1.68	0.92
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:A:354:LEU:HD21	1:A:356:MET:CE	2.01	0.90
1:A:264:THR:HG22	1:A:293:LEU:HD12	1.54	0.90
1:D:21:GLU:CD	2:I:308:SER:HB2	1.97	0.90
1:D:78:MET:HE2	1:D:82:GLU:HG2	1.54	0.89
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:MET:HE1	1:E:342:PHE:CD2	2.09	0.87
1:G:97:MET:HE1	1:G:343:LEU:HD13	1.55	0.86
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:295:GLY:HA3	2:I:446:MET:HE2	1.58	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: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:H:243:PHE:O	1:H:247:GLN:HB3	1.75	0.85
1:B:8:GLU:CD	1:B:74:VAL:HG22	2.01	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:E:122:MET:HE3	1:E:339:LEU:HG	1.59	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:E:284:MET:HE1	1:E:290:ILE:HD11	1.57	0.84
1:D:175:VAL:HG12	1:D:176:LEU:H	1.43	0.83
1:A:131:ALA:HA	1:A:134:MET:HE2	1.60	0.83
1:D:246:LYS:O	1:D:249:GLU:HB3	1.78	0.83
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:G:164:MET:HE1	2:I:370:VAL:HG12	1.61	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:A:354:LEU:HD21	1:A:356:MET:HE2	1.62	0.82
1:G:158:ARG:HB2	1:H:330:ASP:OD2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:MET:H	1:H:122:MET:HE2	1.45	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:E:125:MET:HE3	1:E:134:MET:HB2	1.61	0.80
1:G:163:MET:HB2	1:G:170:VAL:CG1	2.11	0.80
1:A:1:MET:HE2	1:A:1:MET:HA	1.64	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:D:277:THR:H	1:D:280:MET:HE3	1.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:125:MET:HE3	1:D:134:MET:HB2	1.66	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
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:F:324:GLN:HE21	2:F:359:LEU:HD22	1.49	0.76
1:G:203:VAL:HG23	1:G:204:ARG:N	2.00	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:A:277:THR:H	1:A:280:MET:HE2	1.50	0.76
1:G:118:THR:HA	1:G:369:THR:O	1.85	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
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:E:134:MET:HE2	1:E:342:PHE:HA	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:208:LYS:HD2	1:D:208:LYS:C	2.12	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:G:243:PHE:C	1:G:245:LYS:H	1.96	0.74
1:B:1:MET:HE2	1:B:353:THR:HA	1.67	0.74
1:B:369:THR:HB	1:B:374:ILE:HA	1.68	0.74
1:D:164:MET:HE2	1:D:169:THR:HG23	1.67	0.74
1:A:165:THR:HG22	2:C:353:PRO:HB3	1.70	0.74
1:A:276:ILE:HA	1:A:280:MET:HE3	1.68	0.74
1:A:368:VAL:HA	1:A:376:HIS:HB2	1.69	0.74
2:I:425:LYS:HD3	2:I:427:SER:O	1.88	0.74
1:A:354:LEU:HD21	1:A:356:MET:HE1	1.69	0.73
1:E:1:MET:HE3	1:E:30:GLY:O	1.88	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:G:105:ASN:C	1:G:107:PRO:HD2	2.14	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
1:H:61:ALA:O	1:H:89:LEU:HB3	1.90	0.72
1:H:129:SER:HA	1:H:132:GLN:CD	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:MET:HE3	1:A:339:LEU:HD22	1.72	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
2:F:334:LEU:HD12	2:F:463:MET:HE1	1.73	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:I:318:MET:HE3	2:I:324:GLN:H	1.54	0.71
2:C:322:GLN:NE2	2:C:324:GLN:HE22	1.89	0.71
1:G:186:GLN:NE2	1:H:163:MET:HE2	2.05	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:E:284:MET:HE3	1:E:315:VAL:HG21	1.72	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:D:225:ALA:C	1:D:227:LYS:H	1.97	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
2:C:459:ILE:HG22	2:C:463:MET:HE2	1.71	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
2:I:401:THR:C	2:I:403:PRO:HD3	2.15	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:HD11	1:A:356:MET:HE1	1.74	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:D:354:LEU:C	1:D:355:VAL:HG22	2.16	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: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
1:G:330:ASP:OD1	1:H:158:ARG:HD2	1.91	0.69
1:E:118:THR:HA	1:E:369:THR:O	1.93	0.69
2:I:432:TYR:C	2:I:434:GLY:H	1.98	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:G:359:GLU:CD	1:G:359:GLU:H	1.99	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: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
1:E:199:MET:HE3	1:E:254:GLU:OE1	1.93	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:A:304:SER:O	1:A:305:GLU:C	2.36	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:C:330:MET:HG3	2:C:463:MET:HE1	1.77	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:C:464:ASN:C	2:C:464:ASN:ND2	2.48	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:E:86:GLU:C	1:E:88:ALA:H	2.03	0.67
1:B:244:ARG:H	1:B:244:ARG:HD3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:459:ILE:HG22	2:I:463:MET:HE3	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:72:TRP:HE1	1:G:97:MET:HE3	1.60	0.67
1:G:278:GLU:O	1:G:282:THR:HG23	1.95	0.67
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
1:B:97:MET:HE1	1:B:343:LEU:HD12	1.76	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:D:163:MET:HE1	1:E:142:ASN:ND2	2.07	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: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:H:346:HIS:HB3	1:H:356:MET:HB3	1.78	0.66
1:E:348:ASP:CG	1:E:351:THR:HB	2.20	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:B:134:MET:HE3	1:B:342:PHE:HD1	1.60	0.65
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:64:ALA:C	1:H:65:LEU:HD12	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:VAL:O	1:D:115:ARG:CD	2.44	0.65
1:D:285:LYS:HD3	1:D:285:LYS:C	2.22	0.65
1:A:164:MET:HE3	2:C:357:ASN:OD1	1.96	0.65
2:C:433:ALA:O	2:C:435:VAL:HG23	1.96	0.65
1:D:1:MET:HE2	1:D:354:LEU:HB3	1.78	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:H:136:ILE:HG13	1:H:137:LEU:H	1.61	0.65
1:B:164:MET:HA	1:B:164:MET:CE	2.22	0.65
1:D:280:MET:C	1:D:282:THR:H	2.05	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:E:360:ASP:CG	1:E:362:THR:HG22	2.21	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
2:C:373:LEU:HD23	2:C:373:LEU:C	2.22	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
2:I:330:MET:HG3	2:I:463:MET:HE1	1.78	0.65
1:A:136:ILE:HG13	1:A:137:LEU:N	2.12	0.65
1:G:5:ILE:HB	1:G:35:VAL:HG12	1.79	0.65
1:D:91:LYS:O	1:D:92:GLU:C	2.40	0.64
2:F:304:MET:HG2	2:F:385:VAL:HG11	1.79	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:28:GLY:C	1:H:29:LEU:HD12	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:66:SER:O	1:G:91:LYS:HB3	1.98	0.64
1:H:347:VAL:C	1:H:355:VAL:HG12	2.23	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
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
2:F:437:ASN:C	2:F:439:LEU:H	2.06	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
2:F:446:MET:HE3	2:F:448:LEU:CD2	2.27	0.63
1:G:163:MET:HE3	1:G:170:VAL:HG11	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:ILE:CD1	1:E:56:THR:HB	2.28	0.62
2:F:373:LEU:HD23	2:F:373:LEU:C	2.24	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:G:5:ILE:HD12	1:G:5:ILE:N	2.14	0.62
1:B:100:LEU:C	1:B:102:ALA:N	2.55	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:H:67:GLN:H	1:H:67:GLN:CD	2.07	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:151:ASP:CG	1:D:326:ARG:HH21	2.08	0.62
1:D:178:PHE:CE2	1:D:276:ILE:HD11	2.35	0.62
1:B:252:LEU:O	1:B:256:VAL:HG23	2.00	0.61
1:G:186:GLN:CD	1:H:163:MET:HE2	2.24	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
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:G:72:TRP:NE1	1:G:97:MET:HE3	2.15	0.61
1:H:60:THR:HG23	1:H:63:GLN:H	1.63	0.61
1:H:202:ASP:CG	4:H:400:NAD:H8A	2.25	0.61
2:I:304:MET:C	2:I:306:ASN:H	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:199:MET:HE2	1:B:217:LYS:HB3	1.80	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:A:163:MET:HE3	1:A:170:VAL:CG1	2.27	0.61
1:D:5:ILE:HG12	1:D:18:ILE:HB	1.82	0.61
1:D:50:LEU:C	1:D:55:ALA:HB3	2.25	0.61
1:D:276:ILE:HA	1:D:280:MET:HE3	1.82	0.61
1:G:36:GLU:OE1	1:G:61:ALA:HB2	2.01	0.61
1:H:243:PHE:C	1:H:245:LYS:H	2.08	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
1:H:124:LEU:O	1:H:125:MET:C	2.44	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:275:LEU:O	1:D:280:MET:HE1	2.01	0.61
1:G:162:MET:HE3	2:I:357:ASN:ND2	2.15	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:E:281:VAL:HA	1:E:284:MET:HE2	1.84	0.60
1:B:1:MET:CE	1:B:353:THR:HA	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:451:ASP:O	2:I:452:ALA:C	2.44	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:A:376:HIS:CD2	1:A:378:ALA:H	2.19	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: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:I:439:LEU:C	2:I:441:PHE:H	2.08	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
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:B:146:TYR:CE2	1:B:150:ILE:HG13	2.37	0.59
1:E:97:MET:HB3	1:E:122:MET:HE2	1.83	0.59
1:H:5:ILE:HG13	1:H:72:TRP:HD1	1.68	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:8:GLU:H	1:H:8:GLU:CD	2.09	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:122:MET:HE3	1:D:339:LEU:CD2	2.32	0.59
1:G:128:ILE:HD12	1:G:129:SER:H	1.67	0.59
1:H:162:MET:HE2	1:H:164:MET:SD	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:280:MET:C	1:G:282:THR:H	2.10	0.59
1:H:4:ALA:O	1:H:71:VAL:HG23	2.03	0.59
1:D:18:ILE:HD13	1:D:18:ILE:C	2.28	0.59
1:D:357:LYS:C	1:D:359:GLU:H	2.10	0.59
1:E:9:ARG:O	1:E:10:ARG:C	2.45	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: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
1:E:121:ALA:HB1	1:E:123:GLU:CD	2.28	0.59
2:I:346:HIS:CD2	2:I:394:VAL:HB	2.38	0.59
1:A:21:GLU:H	1:A:21:GLU:CD	2.10	0.58
2:F:356:MET:HE2	2:F:356:MET:HA	1.85	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
2:I:295:GLY:CA	2:I:446:MET:HE2	2.31	0.58
2:I:299:ASP:HB3	2:I:446:MET:HE1	1.86	0.58
1:A:140:GLN:C	1:A:142:ASN:H	2.11	0.58
1:E:89:LEU:HD12	1:E:89:LEU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:ALA:C	1:D:207:THR:H	2.11	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
2:F:348:VAL:HG21	2:F:410:MET:HE2	1.85	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:D:122:MET:C	1:D:124:LEU:H	2.11	0.58
1:E:176:LEU:HD23	1:E:199:MET:O	2.02	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
2:C:446:MET:HE3	1:H:164:MET:CE	2.34	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
2:F:374:GLU:H	2:F:374:GLU:CD	2.11	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
2:I:313:VAL:HB	2:I:388:VAL:HG22	1.86	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:124:LEU:HD13	1:H:365:GLY:O	2.04	0.57
1:H:125:MET:HA	1:H:125:MET:HE3	1.84	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:H:330:ASP:C	1:H:333:PRO:HD2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:86:GLU:C	1:E:88:ALA:N	2.61	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:G:273:PRO:HG3	4:G:400:NAD:C2A	2.34	0.57
1:D:4:ALA:HB1	1:D:34:ILE:O	2.04	0.57
1:D:342:PHE:C	1:D:345:PRO:HD2	2.29	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
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:G:370:ARG:O	1:G:371:ASP:C	2.46	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:294:ALA:C	1:H:296:GLU:H	2.12	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:38:GLY:H	1:H:47:ASP:CG	2.12	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
1:D:222:ASP:HB2	1:D:227:LYS:HE2	1.86	0.56
1:E:136:ILE:HD12	1:E:136:ILE:C	2.30	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
1:H:96:LEU:C	1:H:96:LEU:HD23	2.30	0.56
2:I:310:VAL:HG22	2:I:385:VAL:HB	1.86	0.56
1:A:125:MET:HE1	1:A:342:PHE:CD1	2.40	0.56
1:A:178:PHE:HB3	1:A:275:LEU:HD13	1.87	0.56
1:D:175:VAL:HG12	1:D:176:LEU:N	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:MET:C	1:H:124:LEU:H	2.13	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: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: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:330:MET:HE1	2:I:387:PHE:CZ	2.41	0.56
2:I:453:LYS:HE2	2:I:457:GLU:CD	2.31	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:B:100:LEU:C	1:B:102:ALA:H	2.13	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
2:F:407:ILE:O	2:F:408:TYR:C	2.49	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
2:I:432:TYR:C	2:I:434:GLY:N	2.64	0.56
1:A:277:THR:C	1:A:279:GLU:N	2.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:MET:CE	1:E:134:MET:HB2	2.34	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:A:131:ALA:HA	1:A:134:MET:CE	2.33	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
1:E:284:MET:CE	1:E:290:ILE:HD11	2.32	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:C:346:HIS:CD2	2:C:373:LEU:HD12	2.41	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:129:SER:C	1:H:132:GLN:HG3	2.31	0.55
1:H:295:VAL:O	1:H:295:VAL:HG22	2.06	0.55
2:I:433:ALA:C	2:I:435:VAL:H	2.14	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:E:279:GLU:O	1:E:282:THR:OG1	2.20	0.55
1:G:164:MET:CE	2:I:370:VAL:HG12	2.36	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:D:252:LEU:C	1:D:254:GLU:H	2.13	0.55
1:E:212:GLU:C	1:E:214:LEU:N	2.63	0.55
1:H:33:VAL:O	1:H:34:ILE:HD12	2.06	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:330:MET:HE1	2:I:387:PHE:CE2	2.42	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:D:68:ALA:C	1:D:91:LYS:HD3	2.29	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:D:252:LEU:C	1:D:252:LEU:HD23	2.32	0.55
1:E:108:VAL:O	1:E:112:LEU:HD12	2.07	0.55
1:H:297:ALA:C	1:H:299:GLY:H	2.15	0.55
2:C:420:THR:HB	1:H:162:MET:HE1	1.90	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: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
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:G:243:PHE:C	1:G:245:LYS:N	2.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:360:ASP:CG	1:D:362:THR:HB	2.33	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:138:SER:C	1:A:140:GLN:H	2.16	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:D:277:THR:N	1:D:280:MET:HE3	2.21	0.54
1:G:299:GLY:C	1:G:301:CYS:H	2.15	0.54
1:B:255:LEU:HD21	1:B:284:MET:HE2	1.90	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:H:61:ALA:C	1:H:65:LEU:HD13	2.32	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
1:H:135:ASP:OD2	1:H:135:ASP:C	2.50	0.54
2:I:309:LYS:O	2:I:384:ASP:HB2	2.08	0.54
2:C:350:GLY:C	6:C:500:NDP:H71N	2.16	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
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: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:B:339:LEU:O	1:B:340:LEU:C	2.50	0.53
1:D:343:LEU:HD23	1:D:343:LEU:C	2.33	0.53
1:D:354:LEU:C	1:D:354:LEU:HD23	2.32	0.53
1:G:62:ALA:HB2	1:G:89:LEU:CD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:VAL:HG12	1:H:243:PHE:CZ	2.44	0.53
1:H:357:LYS:C	1:H:359:GLU:H	2.16	0.53
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: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:D:285:LYS:HZ2	1:E:44:SER:HB3	1.72	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
2:I:437:ASN:C	2:I:439:LEU:H	2.17	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:D:239:MET:HE2	1:D:243:PHE:CE2	2.43	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:90:ILE:O	1:B:91:LYS:C	2.50	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:G:354:LEU:HD23	1:G:354:LEU:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ASP:OD1	1:D:203:VAL:N	2.41	0.53
1:D:330:ASP:CG	1:E:158:ARG:HG2	2.33	0.53
1:E:214:LEU:HD21	2:F:355:HIS:CD2	2.44	0.53
1:G:62:ALA:CB	1:G:89:LEU:HD23	2.37	0.53
1:G:128:ILE:HD12	1:G:129:SER:N	2.23	0.53
1:H:121:ALA:HB1	1:H:123:GLU:CD	2.32	0.53
1:H:245:LYS:C	1:H:247:GLN:H	2.16	0.53
1:H:354:LEU:O	1:H:356:MET:HE3	2.07	0.53
2:I:445:THR:HG22	2:I:447:MET:HE2	1.91	0.53
1:D:123:GLU:HG2	1:D:124:LEU:HD13	1.89	0.53
1:D:340:LEU:C	1:D:340:LEU:HD23	2.33	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: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: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: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
2:C:321:ALA:O	2:C:322:GLN:HB2	2.08	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:A:21:GLU:CD	1:A:21:GLU:N	2.68	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:G:332:SER:O	1:G:333:PRO:C	2.53	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:B:273:PRO:HG3	4:B:400:NAD:N6A	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:444:ASN:C	2:C:444:ASN:HD22	2.17	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
2:F:445:THR:HG22	2:F:446:MET:N	2.24	0.52
1:B:73:LYS:HZ1	1:B:77:PRO:N	2.07	0.52
1:D:308:LYS:HG2	1:D:309:ILE:N	2.23	0.52
1:E:220:THR:O	1:E:221:VAL:C	2.52	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: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:125:MET:HE3	1:E:134:MET:SD	2.50	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
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:D:354:LEU:C	1:D:355:VAL:CG2	2.83	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: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:405:SER:C	2:F:407:ILE:H	2.18	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
2:I:324:GLN:HG2	2:I:325:HIS:H	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:MET:HE3	1:B:339:LEU:HD11	1.91	0.52
1:B:134:MET:HE1	1:B:362:THR:HG21	1.92	0.52
1:B:184:GLY:O	1:B:187:ALA:HB3	2.10	0.52
2:C:309:LYS:HZ1	2:C:382:THR:HB	1.74	0.52
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
1:A:28:GLY:C	1:A:30:GLY:H	2.17	0.51
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: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:122:MET:HE3	1:B:339:LEU:CD1	2.40	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:A:355:VAL:O	1:A:355:VAL:HG13	2.10	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
1:G:72:TRP:CD1	1:G:97:MET:HE3	2.45	0.51
1:G:208:LYS:O	1:G:212:GLU:HG3	2.09	0.51
1:H:103:LEU:HD11	1:H:124:LEU:HD21	1.91	0.51
1:H:128:ILE:O	1:H:132:GLN:CG	2.58	0.51
2:I:380:PHE:CZ	2:I:413:LEU:HD22	2.44	0.51
2:C:423:PHE:C	2:C:424:ILE:HD12	2.35	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:B:244:ARG:H	1:B:244:ARG:CD	2.24	0.51
2:C:304:MET:HE1	2:C:387:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:HE3	1:D:339:LEU:HD22	1.93	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
1:A:211:VAL:HG12	1:A:212:GLU:N	2.25	0.51
1:A:277:THR:H	1:A:280:MET:HE3	1.76	0.51
1:B:281:VAL:HA	1:B:284:MET:HE3	1.93	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:G:114:LYS:C	1:G:116:LYS:H	2.18	0.51
1:H:1:MET:HE2	1:H:30:GLY:O	2.11	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
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:97:MET:HB2	1:D:122:MET:CE	2.27	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:91:LYS:C	1:D:92:GLU:O	2.52	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:264:THR:O	1:H:265:ALA:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:357:LYS:HB3	1:H:360:ASP:CB	2.34	0.50
2:I:389:ILE:HG23	2:I:389:ILE:O	2.10	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
2:C:446:MET:HE3	1:H:164:MET:HE3	1.92	0.50
1:H:65:LEU:HD12	1:H:65:LEU:N	2.26	0.50
2:I:304:MET:C	2:I:306:ASN:N	2.63	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: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: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:H:98:CYS:H	1:H:122:MET:HE1	1.75	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:D:351:THR:O	1:D:352:LYS:C	2.53	0.50

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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	0.50
2:I:304:MET:HE1	2:I:387:PHE:CE1	2.47	0.50
1:B:134:MET:HG2	1:B:342:PHE:H	1.75	0.50
1:B:147:ARG:HH11	1:B:151:ASP:CG	2.19	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: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
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:208:LYS:NZ	1:G:220:THR:HG23	2.27	0.50
1:H:180:VAL:HG21	1:H:211:VAL:CG2	2.41	0.50
1:H:204:ARG:C	1:H:206:ALA:H	2.20	0.50
1:A:164:MET:HE1	2:C:357:ASN:HD21	1.77	0.50
1:B:87:VAL:C	1:B:89:LEU:H	2.20	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:H:65:LEU:O	1:H:66:SER:C	2.53	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:B:29:LEU:HD21	1:B:344:THR:HB	1.93	0.50
1:B:242:GLU:HA	1:B:242:GLU:OE2	2.10	0.50
1:B:354:LEU:C	1:B:354:LEU:HD23	2.36	0.50
2:C:379:SER:O	2:C:380:PHE:C	2.54	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:B:62:ALA:C	1:B:64:ALA:H	2.19	0.50
1:E:97:MET:HE1	1:E:343:LEU:HD12	1.94	0.50
1:E:282:THR:HG22	1:E:313:HIS:CE1	2.47	0.50
1:E:342:PHE:CD1	1:E:342:PHE:C	2.89	0.50
1:H:113:THR:HG23	1:H:369:THR:OG1	2.12	0.50
1:H:125:MET:HE3	1:H:125:MET:CA	2.42	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:A:125:MET:HE3	1:A:134:MET:CB	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:332:ASP:O	2:I:333:VAL:C	2.54	0.49
1:B:156:PHE:CZ	1:B:259:ASP:HB3	2.47	0.49
2:C:446:MET:CE	1:H:164:MET:HE3	2.42	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
2:F:437:ASN:C	2:F:439:LEU:N	2.68	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:H:245:LYS:C	1:H:247:GLN:N	2.70	0.49
1:A:140:GLN:C	1:A:142:ASN:N	2.67	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
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:325:SER:C	1:H:327:VAL:H	2.20	0.49
1:A:22:VAL:HG13	1:A:340:LEU:HD22	1.94	0.49
1:A:184:GLY:O	1:A:188:ILE:HG13	2.13	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:C:330:MET:HG3	2:C:463:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:C	1:D:207:THR:N	2.71	0.49
1:D:360:ASP:C	1:D:362:THR:H	2.18	0.49
1:E:132:GLN:O	1:E:133:SER:C	2.56	0.49
1:E:273:PRO:O	1:E:274:VAL:C	2.55	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:A:277:THR:C	1:A:279:GLU:H	2.20	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
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:344:THR:HA	1:D:347:VAL:CG2	2.43	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:G:26:LEU:O	1:G:31:PHE:HB2	2.12	0.49
1:G:73:LYS:HE3	1:G:75:GLN:O	2.13	0.49
1:G:78:MET:HE2	1:G:84:THR:HG22	1.94	0.49
1:H:75:GLN:O	1:H:76:ARG:C	2.55	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:A:105:ASN:C	1:A:107:PRO:HD2	2.38	0.48
1:B:128:ILE:HG12	1:B:131:ALA:HB3	1.95	0.48
1:D:255:LEU:C	1:D:257:LYS:H	2.19	0.48
2:F:305:LYS:HZ2	2:F:337:GLU:HG3	1.77	0.48
1:G:247:GLN:C	1:G:249:GLU:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:295:VAL:HG13	1:A:296:GLU:N	2.28	0.48
1:A:362:THR:HG22	1:A:363:VAL:N	2.28	0.48
1:B:100:LEU:O	1:B:101:GLY:C	2.56	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: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:10:ARG:HH22	1:H:82:GLU:CD	2.21	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:D:24:LYS:C	1:D:26:LEU:H	2.21	0.48
1:D:85:ASP:OD2	1:D:88:ALA:HB3	2.14	0.48
1:D:239:MET:H	1:D:244:ARG:HH11	1.59	0.48
1:D:255:LEU:C	1:D:257:LYS:N	2.71	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
1:A:143:LEU:HD23	1:B:163:MET:HE1	1.94	0.48
1:A:351:THR:O	1:A:352:LYS:C	2.56	0.48
1:B:85:ASP:OD1	1:B:88:ALA:HB3	2.13	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
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:D:280:MET:C	1:D:282:THR:N	2.69	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:444:ASN:C	2:C:444:ASN:ND2	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:CYS:O	1:H:121:ALA:HA	2.13	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
2:C:418:ALA:O	2:C:419:GLY:C	2.55	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
2:I:330:MET:CG	2:I:463:MET:HE1	2.44	0.48
2:I:440:PHE:CD2	2:I:447:MET:HE1	2.48	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:H:3:ILE:HG23	1:H:33:VAL:HG22	1.95	0.48
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:99:HIS:CD2	1:B:99:HIS:C	2.92	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:E:190:THR:O	1:E:191:ALA:C	2.56	0.48
1:E:370:ARG:O	1:E:371:ASP:C	2.57	0.48
1:G:207:THR:O	1:G:208:LYS:C	2.57	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:A:359:GLU:CD	1:A:359:GLU:H	2.21	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:H:113:THR:C	1:H:115:ARG:H	2.20	0.48
1:A:7:LYS:H	1:A:36:GLU:CG	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:126:PRO:O	1:D:128:ILE:N	2.43	0.47
1:D:249:GLU:C	1:D:249:GLU:CD	2.82	0.47
1:E:120:TYR:HB3	1:E:366:THR:HG22	1.96	0.47
2:F:356:MET:HE2	2:F:356:MET:CA	2.44	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
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: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:A:343:LEU:HD23	1:A:343:LEU:C	2.39	0.47
1:B:325:SER:O	1:B:328:ALA:HB2	2.14	0.47
1:D:322:ASN:HD22	1:D:325:SER:CB	2.16	0.47
2:F:393:ASP:O	2:F:395:THR:N	2.47	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
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
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:210:GLN:H	1:E:210:GLN:HG2	1.37	0.47
1:E:284:MET:HE1	1:E:290:ILE:CD1	2.38	0.47
1:E:325:SER:C	1:E:327:VAL:H	2.23	0.47
2:F:334:LEU:HB3	2:F:339:VAL:HB	1.96	0.47
1:G:97:MET:HE1	1:G:343:LEU:CD1	2.36	0.47
1:G:188:ILE:CG2	1:G:214:LEU:HD13	2.44	0.47
1:G:346:HIS:CE1	1:G:363:VAL:CG2	2.98	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:143:LEU:CD2	1:B:163:MET:HE1	2.44	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
1:B:348:ASP:CG	1:B:351:THR:HB	2.40	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:231:THR:O	1:D:232:ALA:C	2.58	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:G:199:MET:HE1	1:G:217:LYS:HB2	1.96	0.47
1:H:98:CYS:N	1:H:122:MET:HE1	2.29	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
1:A:15:ARG:NH1	1:A:324:PRO:HB2	2.30	0.47
1:A:277:THR:N	1:A:280:MET:CE	2.70	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:D:193:ARG:C	1:D:195:GLY:H	2.22	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:D:247:GLN:C	1:D:249:GLU:H	2.23	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:A:125:MET:HE3	1:A:134:MET:HB2	1.96	0.47
1:A:327:VAL:O	1:A:328:ALA:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:THR:HB	1:H:162:MET:HE3	1.97	0.47
1:D:94:ALA:O	1:D:117:ILE:HG23	2.15	0.47
1:D:285:LYS:HZ3	1:D:286:PRO:HG2	1.77	0.47
1:D:358:LEU:CD1	1:D:370:ARG:HH22	2.18	0.47
1:E:121:ALA:C	1:E:366:THR:HG23	2.40	0.47
1:E:169:THR:CG2	1:E:170:VAL:N	2.77	0.47
1:G:128:ILE:C	1:G:130:ARG:H	2.23	0.47
1:G:248:ALA:HB1	1:G:280:MET:HE3	1.96	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: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
1:E:138:SER:O	1:E:139:SER:C	2.58	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:H:370:ARG:O	1:H:371:ASP:C	2.57	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:415:VAL:C	2:C:417:LYS:H	2.23	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
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
1:G:199:MET:HE3	1:G:217:LYS:HB2	1.97	0.46
1:G:252:LEU:CD2	1:G:280:MET:HE2	2.46	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:A:342:PHE:CD2	1:A:342:PHE:C	2.93	0.46
1:D:4:ALA:CB	1:D:34:ILE:HB	2.45	0.46
1:D:204:ARG:C	1:D:206:ALA:N	2.73	0.46
1:D:294:ALA:C	1:D:299:GLY:HA2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:PHE:HB2	1:E:263:THR:HA	1.96	0.46
2:F:298:GLU:CD	2:F:298:GLU:H	2.22	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:NZ	2:C:425:LYS:CB	2.79	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:365:VAL:O	2:F:366:PRO:C	2.59	0.46
2:F:452:ALA:H	6:F:500:NDP:C2A	2.28	0.46
2:I:363:ALA:O	2:I:364:ASN:HB2	2.14	0.46
2:I:453:LYS:HE2	2:I:457:GLU:OE2	2.16	0.46
1:B:36:GLU:O	1:B:37:GLN:C	2.58	0.46
1:B:50:LEU:HB3	1:B:55:ALA:HB3	1.97	0.46
1:B:187:ALA:O	1:B:188:ILE:C	2.57	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:280:MET:C	1:G:282:THR:N	2.72	0.46
1:G:373:ALA:O	1:G:375:VAL:HG13	2.16	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:275:LEU:O	1:A:280:MET:HE1	2.15	0.46
1:A:351:THR:HB	1:A:353:THR:HG22	1.98	0.46
1:B:181:GLY:O	1:B:182:VAL:C	2.59	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: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:G:9:ARG:O	1:G:10:ARG:C	2.59	0.46
1:H:5:ILE:HD11	1:H:72:TRP:HE1	1.80	0.46
1:H:284:MET:HE1	1:H:290:ILE:HD11	1.97	0.46
1:A:205:ALA:C	1:A:207:THR:H	2.24	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:212:GLU:C	1:E:214:LEU:H	2.23	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:249:GLU:C	1:H:251:VAL:H	2.23	0.46
1:H:295:VAL:HG11	1:H:319:GLY:CA	2.46	0.46
1:A:120:TYR:HD2	1:A:366:THR:HG22	1.81	0.46
1:A:205:ALA:C	1:A:207:THR:N	2.72	0.46
1:D:120:TYR:CE1	1:D:363:VAL:HG13	2.50	0.46
1:D:122:MET:C	1:D:124:LEU:N	2.74	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:E:343:LEU:C	1:E:343:LEU:HD23	2.41	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:B:299:GLY:C	1:B:301:CYS:H	2.23	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: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:98:CYS:C	1:H:122:MET:HE1	2.41	0.46
1:H:210:GLN:HA	1:H:213:SER:HB3	1.97	0.46
1:H:277:THR:O	1:H:278:GLU:C	2.58	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:G:277:THR:C	1:G:279:GLU:N	2.74	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
1:H:348:ASP:N	1:H:355:VAL:HG12	2.31	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:62:ALA:C	1:B:64:ALA:N	2.72	0.45
1:B:295:VAL:HG11	1:B:320:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:ARG:HD2	2:C:328:ARG:C	2.40	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
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:CE	2.32	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: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:97:MET:HE3	1:E:339:LEU:HD23	1.98	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
2:F:439:LEU:C	2:F:441:PHE:H	2.24	0.45
1:G:265:ALA:HB2	1:G:275:LEU:HD11	1.99	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: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
1:B:360:ASP:C	1:B:360:ASP:OD2	2.58	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:100:LEU:O	1:D:101:GLY:C	2.60	0.45
1:D:100:LEU:C	1:D:102:ALA:N	2.74	0.45
1:D:240:GLY:O	1:D:242:GLU:N	2.49	0.45
2:F:376:ILE:O	2:F:376:ILE:HG12	2.15	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:51:THR:C	1:H:53:ALA:H	2.25	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
2:F:401:THR:OG1	2:F:402:ASP:N	2.48	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
1:B:79:THR:O	1:B:84:THR:O	2.35	0.45
1:D:252:LEU:HD11	1:D:283:LYS:HD3	1.99	0.45
1:E:195:GLY:C	2:I:443:ASN:HD22	2.24	0.45
1:E:267:ILE:HG12	1:E:273:PRO:HD3	1.98	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:252:LEU:C	1:D:254:GLU:N	2.75	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:G:121:ALA:HB1	1:G:123:GLU:CD	2.42	0.45
1:G:360:ASP:O	1:G:361:GLU:C	2.60	0.45
1:A:3:ILE:HG13	1:A:70:VAL:HG13	1.99	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:E:337:LYS:O	1:E:338:ASN:C	2.59	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
2:I:323:ALA:O	2:I:324:GLN:C	2.60	0.45
1:A:122:MET:C	1:A:124:LEU:H	2.24	0.44
1:A:354:LEU:CD2	1:A:356:MET:HE1	2.44	0.44
1:B:105:ASN:O	1:B:108:VAL:HG12	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:TYR:C	1:G:148:ALA:N	2.74	0.44
1:G:337:LYS:O	1:G:338:ASN:C	2.60	0.44
1:G:376:HIS:C	1:G:380:THR:HG22	2.40	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
1:H:356:MET:O	1:H:358:LEU:N	2.50	0.44
2:I:315:GLY:O	2:I:316:TYR:C	2.59	0.44
1:A:18:ILE:N	1:A:336:ALA:HB2	2.32	0.44
1:A:36:GLU:O	1:A:37:GLN:C	2.60	0.44
1:B:199:MET:HE3	1:B:199:MET:HB2	1.90	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: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:H:247:GLN:C	1:H:249:GLU:N	2.75	0.44
1:H:252:LEU:C	1:H:254:GLU:H	2.25	0.44
1:A:167:ALA:HB2	1:B:338:ASN:ND2	2.31	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
2:F:304:MET:C	2:F:306:ASN:N	2.73	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:D:43:ALA:O	1:D:44:SER:HB2	2.18	0.44
1:D:125:MET:HE1	1:D:342:PHE:CD1	2.52	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:A:147:ARG:O	1:A:148:ALA:C	2.58	0.44
1:B:3:ILE:O	1:B:3:ILE:HG23	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:304:MET:HE3	2:F:304:MET:HB2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:GLY:O	1:H:41:VAL:C	2.60	0.44
1:A:161:PRO:HB3	1:B:193:ARG:NH1	2.32	0.44
1:A:277:THR:N	1:A:280:MET:HE3	2.33	0.44
1:A:331:ALA:O	1:A:332:SER:C	2.60	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:225:ALA:C	1:D:227:LYS:N	2.70	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:156:PHE:C	1:E:158:ARG:H	2.26	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
1:H:66:SER:O	1:H:91:LYS:HB2	2.17	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:D:362:THR:O	1:D:362:THR:HG23	2.17	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:278:GLU:HG3	1:G:303:LEU:CD1	2.48	0.44
1:H:24:LYS:C	1:H:26:LEU:H	2.26	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
2:C:298:GLU:N	2:C:298:GLU:CD	2.76	0.44
2:C:380:PHE:C	2:C:382:THR:H	2.26	0.44
1:D:267:ILE:O	1:D:268:PRO:C	2.61	0.44
1:D:357:LYS:C	1:D:359:GLU:N	2.76	0.44
1:E:51:THR:CG2	1:E:57:ILE:HG23	2.48	0.44
2:F:446:MET:CE	2:F:448:LEU:HD21	2.32	0.44
1:G:40:GLY:C	1:G:42:GLY:N	2.75	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
2:I:304:MET:HE1	2:I:387:PHE:HE1	1.81	0.44
1:B:47:ASP:CG	1:B:57:ILE:HD13	2.43	0.44
1:B:121:ALA:HB3	1:B:124:LEU:HD12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:SER:HB3	1:H:22:VAL:HB	2.00	0.44
1:A:38:GLY:H	1:A:47:ASP:CG	2.26	0.43
1:A:134:MET:HG2	1:A:341:ASN:C	2.43	0.43
1:A:175:VAL:HG12	1:A:176:LEU:N	2.33	0.43
1:B:247:GLN:C	1:B:249:GLU:H	2.26	0.43
1:D:109:VAL:CG2	1:D:110:GLU:N	2.81	0.43
1:D:199:MET:HE2	1:D:199:MET:HB2	1.85	0.43
2:F:450:GLY:HA3	2:F:455:MET:HE3	2.00	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:8:GLU:OE1	1:B:74:VAL:HG22	2.15	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:E:143:LEU:C	1:E:145:GLY:N	2.75	0.43
1:G:10:ARG:HG3	1:G:11:PRO:HD2	2.00	0.43
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
1:A:70:VAL:HG23	1:A:97:MET:HE3	2.00	0.43
1:A:360:ASP:C	1:A:362:THR:N	2.76	0.43
2:C:330:MET:HB2	2:C:460:VAL:CG2	2.48	0.43
1:D:28:GLY:C	1:D:30:GLY:N	2.76	0.43
1:D:194:LEU:CD2	1:E:194:LEU:HD13	2.47	0.43
1:D:204:ARG:C	1:D:206:ALA:H	2.26	0.43
1:D:241:GLU:O	1:D:241:GLU:OE2	2.36	0.43
1:D:255:LEU:C	1:D:255:LEU:HD23	2.43	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
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:H:297:ALA:C	1:H:299:GLY:N	2.77	0.43
1:A:91:LYS:O	1:A:92:GLU:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:SER:HA	2:C:406:PRO:HD3	1.73	0.43
2:C:438:GLU:O	2:C:438:GLU:HG2	2.17	0.43
1:D:105:ASN:O	1:D:106:ARG:C	2.61	0.43
1:D:348:ASP:OD2	1:D:353:THR:N	2.46	0.43
1:E:28:GLY:C	1:E:29:LEU:HD12	2.44	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:H:247:GLN:C	1:H:249:GLU:H	2.26	0.43
1:A:216:GLY:C	1:A:217:LYS:HD2	2.43	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
2:C:392:ASN:O	2:C:393:ASP:C	2.61	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: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
2:F:372:GLU:O	2:F:373:LEU:C	2.62	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:106:ARG:O	1:B:107:PRO:C	2.61	0.43
1:D:5:ILE:HD13	1:D:18:ILE:HG13	2.01	0.43
1:D:264:THR:CG2	1:D:293:LEU:HD12	2.44	0.43
1:E:219:ILE:C	1:E:221:VAL:HG22	2.44	0.43
1:E:280:MET:O	1:E:283:LYS:N	2.45	0.43
1:G:26:LEU:O	1:G:29:LEU:HB2	2.18	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
2:C:377:ASN:OD1	2:C:413:LEU:HA	2.19	0.43
2:C:446:MET:HE3	1:H:164:MET:HE2	1.99	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:B:134:MET:HE3	1:B:342:PHE:CD1	2.48	0.43
2:C:351:ARG:C	6:C:500:NDP:H42N	2.44	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:E:122:MET:C	1:E:124:LEU:N	2.77	0.43
1:G:247:GLN:O	1:G:249:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:LEU:HD21	1:H:344:THR:HG22	2.01	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:H:360:ASP:C	1:H:362:THR:N	2.76	0.43
1:A:291:ILE:CD1	1:A:318:VAL:HB	2.40	0.43
1:B:75:GLN:O	1:B:76:ARG:C	2.60	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: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:122:MET:C	1:H:124:LEU:N	2.75	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:A:28:GLY:C	1:A:30:GLY:N	2.74	0.43
1:B:134:MET:HE2	1:B:134:MET:HB2	1.64	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:G:158:ARG:HB2	1:H:330:ASP:CG	2.42	0.43
1:H:285:LYS:HA	1:H:286:PRO:HD3	1.80	0.43
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: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
2:C:385:VAL:HG12	2:C:386:ALA:N	2.32	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:G:376:HIS:C	1:G:378:ALA:H	2.27	0.42
1:H:19:SER:O	1:H:20:PRO:C	2.62	0.42
1:H:65:LEU:HB3	1:H:90:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:H	1:A:36:GLU:CD	2.26	0.42
1:B:199:MET:HE2	1:B:217:LYS:CB	2.48	0.42
1:D:80:ALA:C	1:D:82:GLU:N	2.78	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:H:337:LYS:O	1:H:338:ASN:C	2.61	0.42
1:H:357:LYS:C	1:H:359:GLU:N	2.75	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:B:347:VAL:O	1:B:348:ASP:C	2.63	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: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
2:F:373:LEU:C	2:F:373:LEU:CD2	2.91	0.42
2:F:454:LYS:O	2:F:455:MET:C	2.62	0.42
1:G:97:MET:O	1:G:98:CYS:HB3	2.18	0.42
1:G:351:THR:O	1:G:352:LYS:C	2.61	0.42
1:H:72:TRP:CB	1:H:97:MET:HB2	2.25	0.42
1:H:325:SER:C	1:H:327:VAL:N	2.76	0.42
1:A:40:GLY:C	1:A:42:GLY:N	2.76	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:D:360:ASP:C	1:D:362:THR:N	2.78	0.42
1:E:23:VAL:HG21	1:E:50:LEU:CD1	2.49	0.42
1:G:347:VAL:C	1:G:348:ASP:O	2.63	0.42
1:H:71:VAL:O	1:H:96:LEU:HA	2.20	0.42
1:A:1:MET:HA	1:A:1:MET:CE	2.44	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:192:LYS:C	1:B:194:LEU:N	2.76	0.42
1:B:247:GLN:C	1:B:249:GLU:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LEU:HD12	1:E:112:LEU:N	2.32	0.42
1:E:143:LEU:O	1:E:144:ALA:C	2.61	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
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:H:98:CYS:C	1:H:122:MET:CE	2.93	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:186:GLN:O	1:B:187:ALA:C	2.61	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
2:C:292:HIS:CD2	2:C:292:HIS:C	2.97	0.42
1:D:65:LEU:O	1:D:66:SER:C	2.63	0.42
1:D:120:TYR:CZ	1:D:356:MET:HG2	2.54	0.42
1:E:72:TRP:HE1	1:E:97:MET:CE	2.33	0.42
1:E:106:ARG:N	1:E:107:PRO:CD	2.82	0.42
1:E:199:MET:HE2	1:E:199:MET:HB2	1.89	0.42
1:E:203:VAL:O	1:E:204:ARG:C	2.62	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
2:F:323:ALA:O	2:F:324:GLN:C	2.63	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:37:GLN:O	1:A:38:GLY:C	2.63	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: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
2:I:393:ASP:OD2	6:I:500:NDP:O3D	2.35	0.42
2:I:448:LEU:C	2:I:455:MET:HE3	2.44	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:204:ARG:C	1:B:206:ALA:H	2.27	0.42
2:C:399:ALA:HB2	2:C:407:ILE:CD1	2.49	0.42
1:D:46:THR:O	1:D:47:ASP:C	2.63	0.42
1:D:51:THR:OG1	1:D:57:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:GLU:C	1:D:363:VAL:H	2.27	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
1:A:293:LEU:HD22	1:A:323:VAL:HG21	2.01	0.42
1:A:354:LEU:CD1	1:A:356:MET:HE1	2.47	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
1:B:277:THR:O	1:B:278:GLU:C	2.62	0.42
2:C:394:VAL:HG22	6:C:500:NDP:O1N	2.20	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
2:F:429:ALA:HB3	6:F:500:NDP:O1X	2.18	0.42
1:H:46:THR:OG1	1:H:49:ALA:CB	2.68	0.42
1:H:131:ALA:CA	1:H:134:MET:HE3	2.33	0.42
1:H:294:ALA:C	1:H:296:GLU:N	2.78	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:B:58:ALA:CB	1:B:64:ALA:HA	2.51	0.41
1:B:341:ASN:C	1:B:343:LEU:N	2.75	0.41
2:C:377:ASN:C	2:C:379:SER:H	2.29	0.41
2:C:426:ARG:O	2:C:449:PHE:HD1	2.02	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
2:F:392:ASN:O	2:F:393:ASP:C	2.63	0.41
1:G:208:LYS:O	1:G:209:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:LYS:O	1:H:212:GLU:HB2	2.20	0.41
1:H:316:LYS:C	1:H:317:ILE:HD12	2.46	0.41
2:I:318:MET:HE1	2:I:324:GLN:HB3	2.02	0.41
2:I:428:MET:O	2:I:429:ALA:C	2.62	0.41
1:A:330:ASP:O	1:A:333:PRO:HD2	2.19	0.41
2:C:451:ASP:O	2:C:452:ALA:C	2.63	0.41
1:D:156:PHE:CZ	1:D:259:ASP:HB3	2.55	0.41
1:D:303:LEU:O	1:D:304:SER:C	2.63	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
1:E:8:GLU:CD	1:E:74:VAL:HG22	2.46	0.41
1:E:247:GLN:C	1:E:249:GLU:N	2.78	0.41
1:G:20:PRO:HD3	1:G:45:ILE:HD13	2.03	0.41
1:H:92:GLU:C	1:H:116:LYS:HE2	2.45	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:60:THR:O	1:B:61:ALA:C	2.62	0.41
1:B:106:ARG:HH12	1:B:374:ILE:CD1	2.34	0.41
1:B:126:PRO:C	1:B:128:ILE:H	2.27	0.41
1:E:16:VAL:O	1:E:16:VAL:HG13	2.20	0.41
1:E:334:LEU:O	1:E:335:PHE:C	2.62	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:H:295:VAL:HG11	1:H:319:GLY:C	2.46	0.41
1:A:97:MET:O	1:A:98:CYS:HB3	2.19	0.41
1:B:242:GLU:O	1:B:245:LYS:CB	2.67	0.41
1:D:49:ALA:O	1:D:50:LEU:C	2.63	0.41
1:D:224:GLU:N	1:D:227:LYS:HG2	2.35	0.41
2:F:370:VAL:C	2:F:371:PHE:CD2	2.98	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: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:138:SER:C	1:A:140:GLN:N	2.78	0.41
1:B:147:ARG:O	1:B:148:ALA:C	2.62	0.41
1:B:339:LEU:C	1:B:341:ASN:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ASP:O	1:D:227:LYS:HE3	2.21	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
2:F:318:MET:HE3	2:F:324:GLN:CA	2.51	0.41
2:F:334:LEU:CD1	2:F:463:MET:HE1	2.47	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:86:GLU:O	1:A:87:VAL:C	2.64	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
2:C:331:ALA:O	2:C:335:LYS:HG3	2.20	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
1:B:122:MET:C	1:B:124:LEU:H	2.29	0.41
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:255:LEU:CD2	1:B:284:MET:HE2	2.51	0.41
2:C:424:ILE:N	2:C:424:ILE:CD1	2.82	0.41
1:D:125:MET:CE	1:D:134:MET:HB2	2.44	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:162:MET:HE2	2:I:420:THR:OG1	2.21	0.41
1:E:278:GLU:C	1:E:281:VAL:HG12	2.42	0.41
1:E:358:LEU:H	1:E:358:LEU:CD1	2.15	0.41
1:G:78:MET:HE2	1:G:84:THR:CG2	2.51	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:H:25:LYS:HE3	1:H:25:LYS:CA	2.51	0.41
1:H:322:ASN:O	1:H:323:VAL:C	2.63	0.41
1:A:299:GLY:C	1:A:301:CYS:H	2.27	0.41
1:A:340:LEU:HD12	1:A:340:LEU:HA	1.77	0.41
1:B:337:LYS:C	1:B:339:LEU:N	2.79	0.41
1:B:337:LYS:O	1:B:338:ASN:C	2.63	0.41
2:C:414:ASP:HB3	2:C:417:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:446:MET:SD	1:H:164:MET:HE3	2.61	0.41
1:D:8:GLU:CD	1:D:74:VAL:HB	2.46	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:D:346:HIS:HB2	1:D:356:MET:HE3	2.03	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:247:GLN:C	1:E:249:GLU:H	2.28	0.41
1:E:311:VAL:O	1:E:311:VAL:HG13	2.20	0.41
2:F:352:MET:HE3	2:F:353:PRO:O	2.21	0.41
2:F:393:ASP:C	2:F:395:THR:H	2.28	0.41
2:F:425:LYS:HB2	6:F:500:NDP:O2X	2.21	0.41
2:F:439:LEU:C	2:F:441:PHE:N	2.79	0.41
1:G:176:LEU:HG	1:G:199:MET:HB3	2.03	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:204:ARG:C	1:H:206:ALA:N	2.76	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
1:B:332:SER:C	1:B:334:LEU:N	2.80	0.41
2:C:373:LEU:C	2:C:373:LEU:CD2	2.91	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
1:E:84:THR:HG23	1:E:84:THR:O	2.20	0.41
1:E:90:ILE:O	1:E:91:LYS:C	2.64	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
2:F:355:HIS:C	2:F:356:MET:HE2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:22:VAL:O	1:A:23:VAL:C	2.60	0.40
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:96:LEU:HD23	1:D:96:LEU:C	2.46	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:G:170:VAL:HG23	1:H:330:ASP:CG	2.46	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:D:181:GLY:O	1:D:182:VAL:C	2.64	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:208:LYS:O	1:A:212:GLU:HG3	2.21	0.40
1:A:284:MET:HE2	1:A:288:SER:HB3	2.03	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
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:E:122:MET:C	1:E:124:LEU:H	2.30	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:100:LEU:O	1:G:101:GLY:C	2.63	0.40
1:G:159:ALA:HA	1:H:146:TYR:CE2	2.55	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
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
2:I:379:SER:C	2:I:381:GLN:N	2.77	0.40
1:A:18:ILE:HD11	1:A:23:VAL:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:120:TYR:CZ	1:B:356:MET:HE2	2.57	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
2:C:407:ILE:O	2:C:408:TYR:C	2.64	0.40
1:D:1:MET:HE2	1:D:354:LEU:CB	2.50	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: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:E:253:LYS:HE3	1:E:253:LYS:C	2.43	0.40
1:E:280:MET:C	1:E:282:THR:N	2.78	0.40
1:G:7:LYS:CG	1:G:39:ALA:HA	2.51	0.40
1:G:27:VAL:C	1:G:29:LEU:N	2.77	0.40
1:G:69:ASP:O	1:G:94:ALA:HB1	2.22	0.40
1:G:99:HIS:C	1:G:99:HIS:ND1	2.79	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%)	1	10
1	B	355/384 (92%)	273 (77%)	57 (16%)	25 (7%)	1	5
1	D	376/384 (98%)	277 (74%)	66 (18%)	33 (9%)	0	3
1	E	355/384 (92%)	265 (75%)	66 (19%)	24 (7%)	1	5
1	G	360/384 (94%)	292 (81%)	50 (14%)	18 (5%)	1	11
1	H	353/384 (92%)	258 (73%)	77 (22%)	18 (5%)	1	10
2	C	172/174 (99%)	133 (77%)	35 (20%)	4 (2%)	5	23
2	F	171/174 (98%)	141 (82%)	21 (12%)	9 (5%)	1	10
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	6

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

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Mol	Chain	Res	Type
2	I	378	SER
2	I	402	ASP
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

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Mol	Chain	Res	Type
1	B	37	GLN
1	B	88	ALA
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

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Mol	Chain	Res	Type
1	B	349	LYS
1	D	74	VAL
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

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Mol	Chain	Res	Type
1	G	375	VAL
1	G	377	PRO
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 ⓘ

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%)	249 (88%)	35 (12%)	4	20
1	B	281/296 (95%)	254 (90%)	27 (10%)	8	30
1	D	293/296 (99%)	251 (86%)	42 (14%)	3	14
1	E	281/296 (95%)	252 (90%)	29 (10%)	7	27
1	G	284/296 (96%)	254 (89%)	30 (11%)	6	26
1	H	280/296 (95%)	234 (84%)	46 (16%)	2	11
2	C	138/138 (100%)	123 (89%)	15 (11%)	6	24
2	F	137/138 (99%)	128 (93%)	9 (7%)	15	43
2	I	137/138 (99%)	129 (94%)	8 (6%)	18	48
All	All	2115/2190 (97%)	1874 (89%)	241 (11%)	5	23

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	41	VAL
1	A	46	THR
1	A	51	THR
1	A	60	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	113	THR
1	A	127	ARG
1	A	164	MET
1	A	170	VAL
1	A	176	LEU
1	A	185	LEU
1	A	199	MET
1	A	203	VAL
1	A	207	THR
1	A	211	VAL
1	A	212	GLU
1	A	217	LYS
1	A	222	ASP
1	A	260	ILE
1	A	270	LYS
1	A	271	PRO
1	A	274	VAL
1	A	344	THR
1	A	348	ASP
1	A	354	LEU
1	A	358	LEU
1	A	362	THR
1	A	366	THR
1	B	10	ARG
1	B	19	SER
1	B	22	VAL
1	B	65	LEU
1	B	71	VAL
1	B	107	PRO
1	B	115	ARG
1	B	130	ARG

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Mol	Chain	Res	Type
1	B	134	MET
1	B	164	MET
1	B	176	LEU
1	B	194	LEU
1	B	217	LYS
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	324	PRO
1	B	344	THR
1	B	347	VAL
1	B	348	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	310	VAL
2	C	358	VAL
2	C	372	GLU
2	C	376	ILE
2	C	379	SER
2	C	382	THR
2	C	416	GLU
2	C	420	THR
2	C	425	LYS
2	C	438	GLU
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	32	GLU

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Mol	Chain	Res	Type
1	D	51	THR
1	D	57	ILE
1	D	65	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
1	D	136	ILE
1	D	137	LEU
1	D	164	MET
1	D	170	VAL
1	D	176	LEU
1	D	177	VAL
1	D	199	MET
1	D	207	THR
1	D	221	VAL
1	D	246	LYS
1	D	249	GLU
1	D	252	LEU
1	D	255	LEU
1	D	268	PRO
1	D	291	ILE
1	D	322	ASN
1	D	343	LEU
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	27	VAL
1	E	57	ILE
1	E	74	VAL
1	E	95	VAL
1	E	96	LEU
1	E	104	THR
1	E	105	ASN

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Mol	Chain	Res	Type
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	244	ARG
1	E	252	LEU
1	E	253	LYS
1	E	258	THR
1	E	270	LYS
1	E	310	VAL
1	E	323	VAL
1	E	330	ASP
1	E	334	LEU
1	E	344	THR
1	E	346	HIS
1	E	348	ASP
1	E	349	LYS
1	E	370	ARG
2	F	293	MET
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	420	THR
1	G	21	GLU
1	G	27	VAL
1	G	31	PHE
1	G	41	VAL
1	G	57	ILE
1	G	60	THR
1	G	63	GLN
1	G	92	GLU
1	G	96	LEU
1	G	128	ILE
1	G	170	VAL
1	G	176	LEU

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Mol	Chain	Res	Type
1	G	177	VAL
1	G	190	THR
1	G	192	LYS
1	G	198	VAL
1	G	199	MET
1	G	220	THR
1	G	222	ASP
1	G	247	GLN
1	G	252	LEU
1	G	255	LEU
1	G	308	LYS
1	G	311	VAL
1	G	334	LEU
1	G	352	LYS
1	G	359	GLU
1	G	361	GLU
1	G	362	THR
1	G	369	THR
1	H	1	MET
1	H	15	ARG
1	H	22	VAL
1	H	25	LYS
1	H	26	LEU
1	H	34	ILE
1	H	35	VAL
1	H	37	GLN
1	H	67	GLN
1	H	72	TRP
1	H	76	ARG
1	H	90	ILE
1	H	97	MET
1	H	105	ASN
1	H	112	LEU
1	H	125	MET
1	H	137	LEU
1	H	147	ARG
1	H	158	ARG
1	H	164	MET
1	H	170	VAL
1	H	176	LEU
1	H	192	LYS
1	H	194	LEU

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Mol	Chain	Res	Type
1	H	244	ARG
1	H	247	GLN
1	H	252	LEU
1	H	258	THR
1	H	277	THR
1	H	278	GLU
1	H	279	GLU
1	H	281	VAL
1	H	289	VAL
1	H	291	ILE
1	H	306	PRO
1	H	310	VAL
1	H	318	VAL
1	H	327	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	142	ASN
1	A	186	GLN
1	A	247	GLN
1	A	376	HIS
1	B	63	GLN
1	B	99	HIS
1	B	105	ASN

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Mol	Chain	Res	Type
1	B	142	ASN
1	B	186	GLN
1	B	210	GLN
1	B	247	GLN
1	B	313	HIS
1	B	320	HIS
1	B	338	ASN
1	B	341	ASN
1	B	376	HIS
2	C	322	GLN
2	C	325	HIS
2	C	346	HIS
2	C	364	ASN
2	C	444	ASN
2	C	458	GLN
2	C	464	ASN
1	D	75	GLN
1	D	99	HIS
1	D	140	GLN
1	D	142	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	376	HIS
1	E	37	GLN
1	E	63	GLN
1	E	132	GLN
1	E	142	ASN
1	E	186	GLN
1	E	210	GLN
1	E	338	ASN
1	E	341	ASN
1	E	376	HIS
2	F	458	GLN
1	G	37	GLN
1	G	142	ASN
1	G	186	GLN
1	G	338	ASN

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Mol	Chain	Res	Type
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	322	ASN
1	H	376	HIS
2	I	325	HIS
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	1.21	1 (9%)	15,15,17	0.75	1 (6%)
3	FRU	J	2	3	11,12,12	1.45	2 (18%)	10,18,18	0.58	0
3	GLC	K	1	3	11,11,12	1.13	1 (9%)	15,15,17	0.87	1 (6%)
3	FRU	K	2	3	11,12,12	1.52	2 (18%)	10,18,18	0.63	0
3	GLC	L	1	3	11,11,12	1.25	1 (9%)	15,15,17	0.82	1 (6%)
3	FRU	L	2	3	11,12,12	1.51	2 (18%)	10,18,18	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	M	1	3	11,11,12	0.99	1 (9%)	15,15,17	0.82	1 (6%)
3	FRU	M	2	3	11,12,12	1.59	2 (18%)	10,18,18	0.71	0
3	GLC	N	1	3	11,11,12	1.33	1 (9%)	15,15,17	0.88	1 (6%)
3	FRU	N	2	3	11,12,12	1.60	2 (18%)	10,18,18	0.61	0
3	GLC	O	1	3	11,11,12	1.29	1 (9%)	15,15,17	0.81	1 (6%)
3	FRU	O	2	3	11,12,12	1.51	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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	FRU	C4-C5	-4.16	1.42	1.53
3	J	2	FRU	C4-C5	-3.93	1.43	1.53
3	L	2	FRU	C4-C5	-3.86	1.43	1.53
3	N	2	FRU	O2-C2	3.58	1.46	1.40
3	O	2	FRU	C4-C5	-3.56	1.44	1.53
3	K	2	FRU	O2-C2	3.45	1.46	1.40
3	N	2	FRU	C4-C5	-3.41	1.44	1.53
3	K	2	FRU	C4-C5	-3.40	1.44	1.53
3	N	1	GLC	O5-C1	3.36	1.49	1.43
3	O	2	FRU	O2-C2	3.13	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1	GLC	O5-C1	3.12	1.48	1.43
3	L	1	GLC	O5-C1	3.02	1.48	1.43
3	K	1	GLC	O5-C1	2.98	1.48	1.43
3	M	2	FRU	O2-C2	2.98	1.45	1.40
3	L	2	FRU	O2-C2	2.96	1.45	1.40
3	J	1	GLC	O5-C1	2.95	1.48	1.43
3	M	1	GLC	O5-C1	2.65	1.48	1.43
3	J	2	FRU	O2-C2	2.54	1.45	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	GLC	C2-C3-C4	-2.40	106.64	110.86
3	O	1	GLC	C2-C3-C4	-2.33	106.76	110.86
3	L	1	GLC	C2-C3-C4	-2.33	106.76	110.86
3	N	1	GLC	C2-C3-C4	-2.33	106.77	110.86
3	J	1	GLC	C2-C3-C4	-2.31	106.80	110.86
3	K	1	GLC	C2-C3-C4	-2.19	107.02	110.86

There are no chirality outliers.

All (15) torsion outliers are listed below:

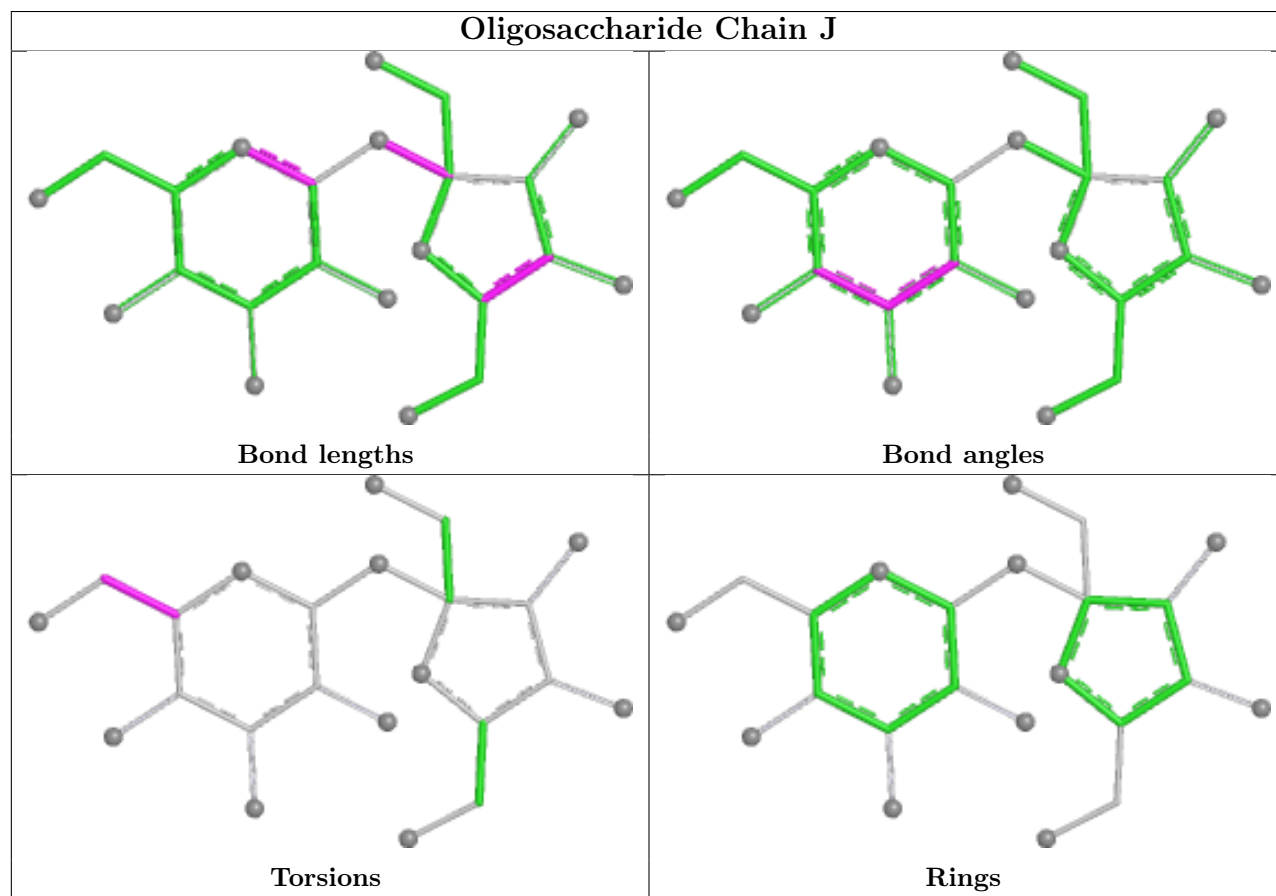
Mol	Chain	Res	Type	Atoms
3	K	2	FRU	C4-C5-C6-O6
3	K	2	FRU	O5-C5-C6-O6
3	N	1	GLC	O5-C5-C6-O6
3	N	2	FRU	C4-C5-C6-O6
3	N	2	FRU	O5-C5-C6-O6
3	N	1	GLC	C4-C5-C6-O6
3	O	2	FRU	O5-C5-C6-O6
3	O	1	GLC	C4-C5-C6-O6
3	J	1	GLC	C4-C5-C6-O6
3	L	1	GLC	C4-C5-C6-O6
3	O	2	FRU	C4-C5-C6-O6
3	O	1	GLC	O5-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6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

There are no ring outliers.

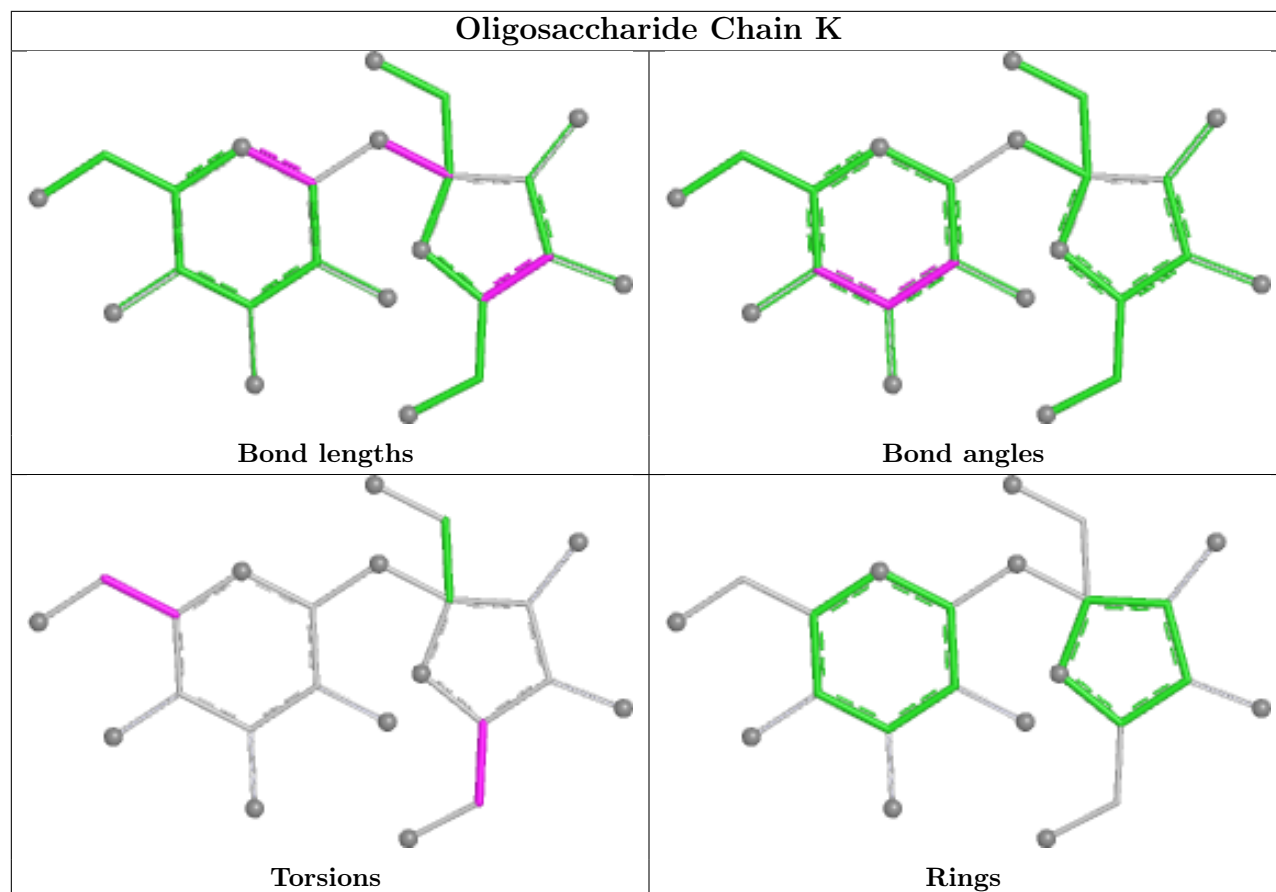
2 monomers are involved in 2 short contacts:

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

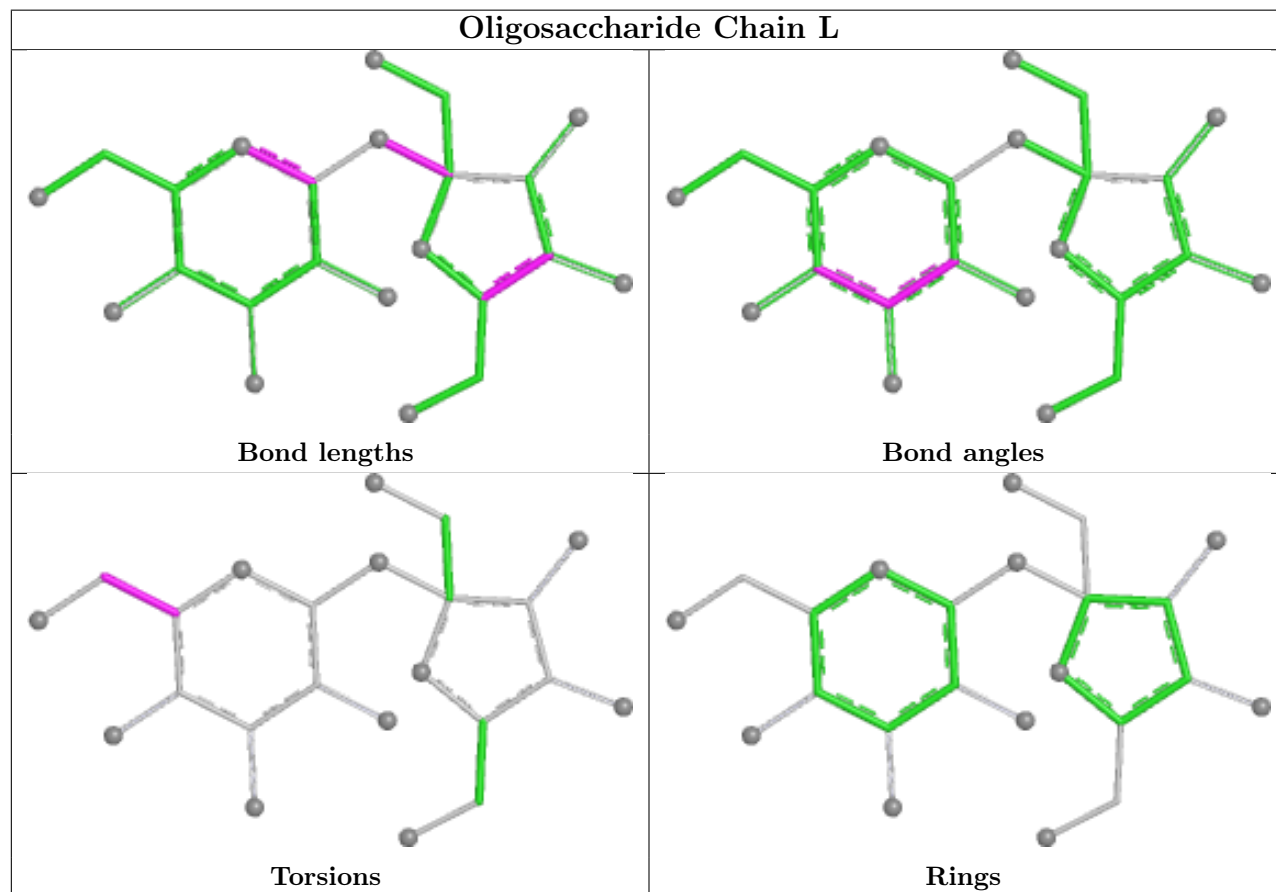
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



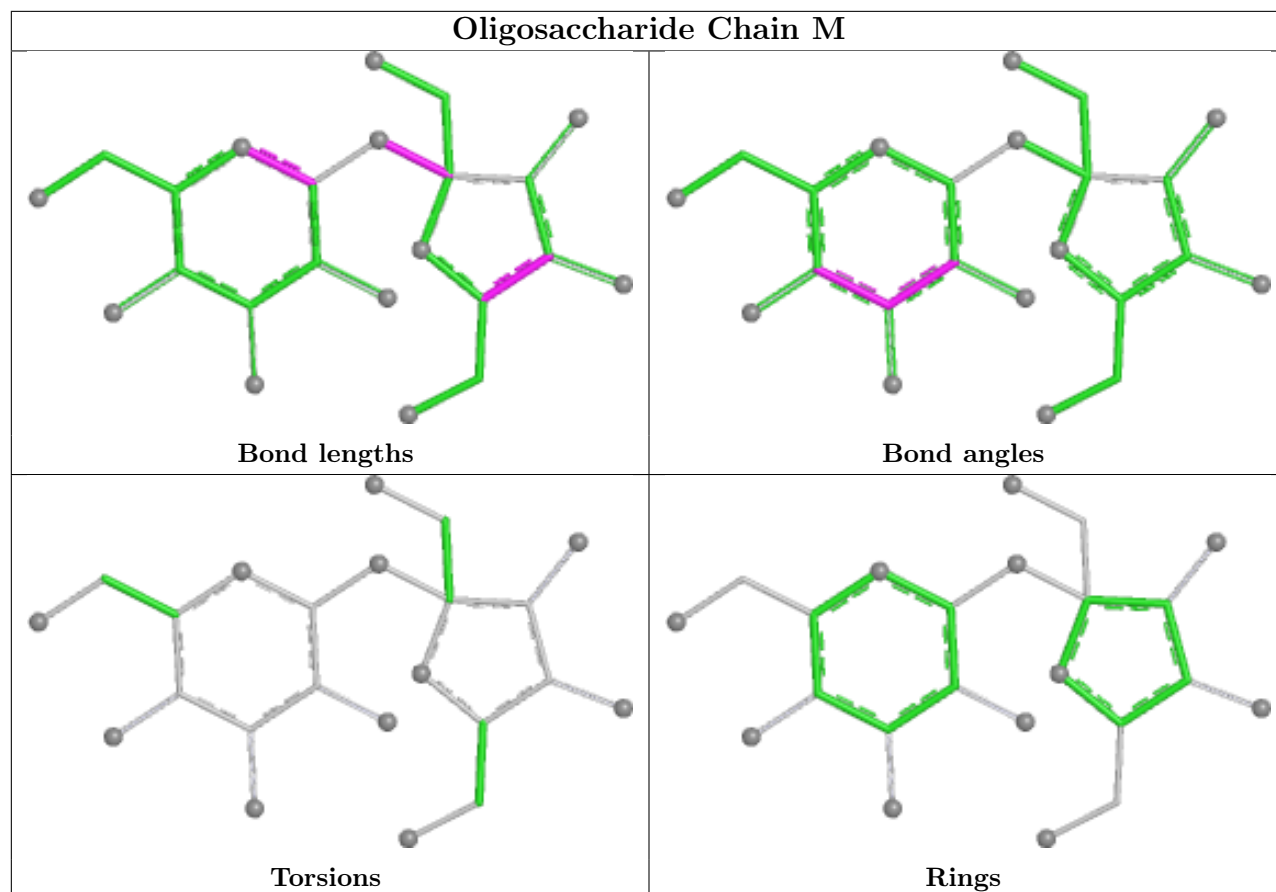
Oligosaccharide Chain K



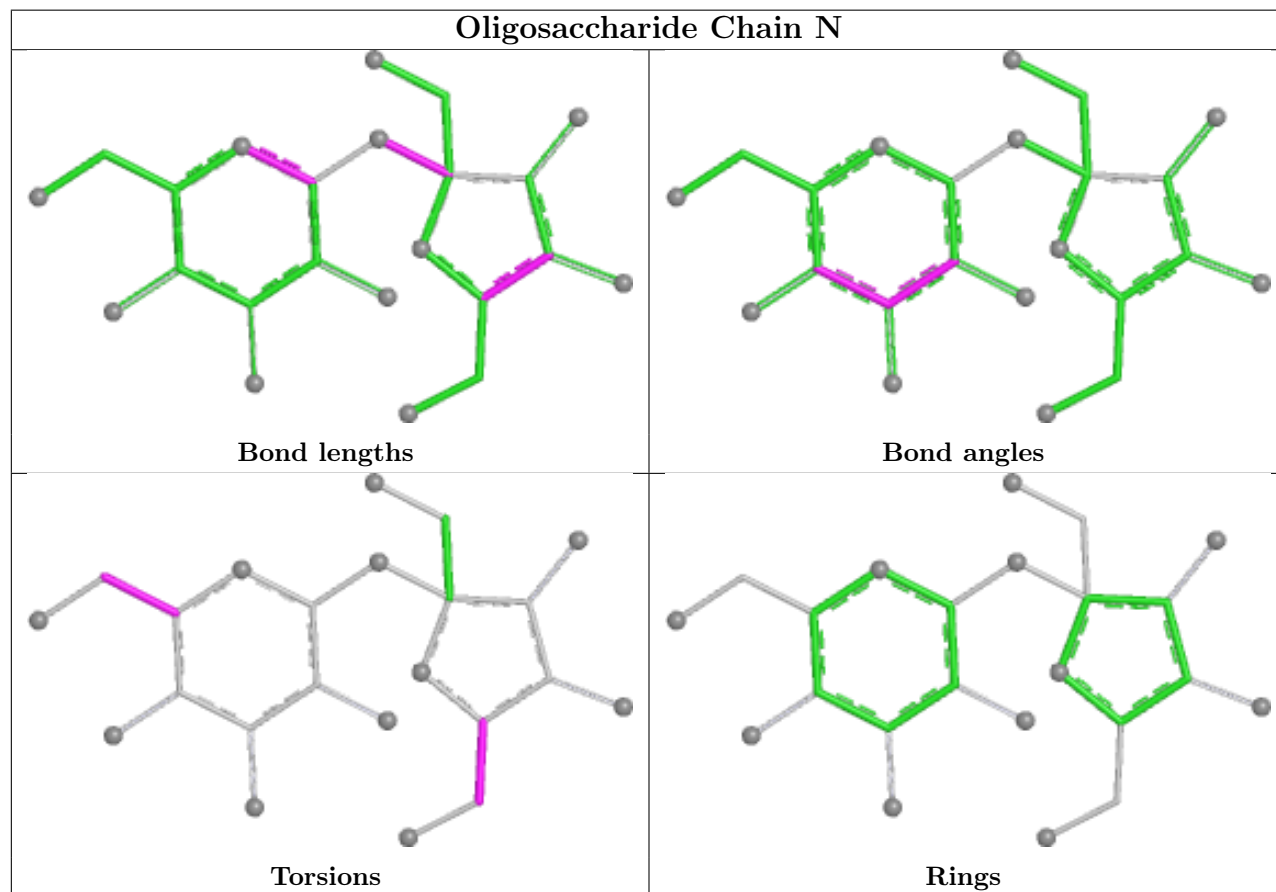
Oligosaccharide Chain L

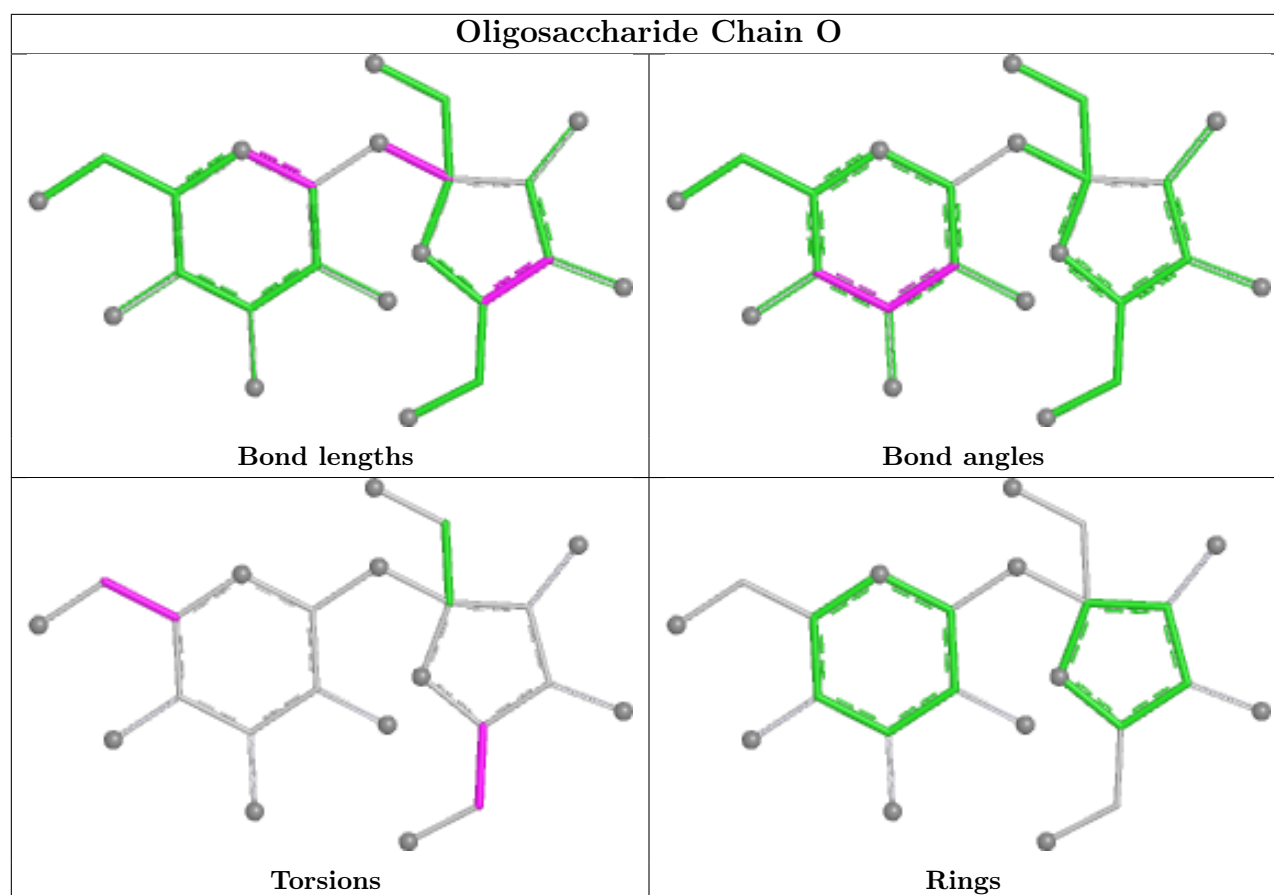


Oligosaccharide Chain M



Oligosaccharide Chain N





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	$\# Z > 2$
6	NDP	F	500	-	51,52,52	2.57	17 (33%)	71,80,80	2.35	32 (45%)
4	NAD	G	400	-	46,48,48	2.82	15 (32%)	64,73,73	2.99	31 (48%)
6	NDP	I	500	-	51,52,52	2.42	16 (31%)	71,80,80	2.35	31 (43%)
4	NAD	D	400	-	46,48,48	2.93	15 (32%)	64,73,73	2.51	30 (46%)
4	NAD	B	400	-	46,48,48	3.14	21 (45%)	64,73,73	2.98	24 (37%)
4	NAD	H	400	-	46,48,48	3.28	16 (34%)	64,73,73	2.56	26 (40%)
4	NAD	A	400	-	46,48,48	2.81	20 (43%)	64,73,73	2.68	33 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NDP	C	500	-	51,52,52	2.36	18 (35%)	71,80,80	2.44	32 (45%)

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
6	NDP	F	500	-	-	13/34/77/77	0/5/5/5
4	NAD	G	400	-	-	9/30/62/62	0/5/5/5
6	NDP	I	500	-	-	10/34/77/77	0/5/5/5
4	NAD	D	400	-	-	10/30/62/62	0/5/5/5
4	NAD	B	400	-	-	16/30/62/62	0/5/5/5
4	NAD	H	400	-	-	13/30/62/62	0/5/5/5
4	NAD	A	400	-	-	15/30/62/62	0/5/5/5
6	NDP	C	500	-	-	13/34/77/77	0/5/5/5

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	400	NAD	PN-O3	-15.08	1.43	1.59
4	B	400	NAD	PN-O3	10.83	1.71	1.59
6	F	500	NDP	PN-O3	10.43	1.70	1.59
4	D	400	NAD	PN-O3	9.87	1.70	1.59
4	G	400	NAD	PN-O3	9.27	1.69	1.59
6	C	500	NDP	PN-O3	8.81	1.69	1.59
6	I	500	NDP	O4D-C1D	8.40	1.61	1.42
4	A	400	NAD	PN-O3	-8.28	1.50	1.59
4	B	400	NAD	C2N-N1N	7.89	1.43	1.35
4	D	400	NAD	C5A-C4A	7.81	1.53	1.39
4	G	400	NAD	C2N-N1N	7.77	1.43	1.35
4	H	400	NAD	C5A-C4A	7.36	1.52	1.39
4	G	400	NAD	C5A-C4A	7.35	1.52	1.39
4	B	400	NAD	C5A-C4A	7.34	1.52	1.39
6	I	500	NDP	C5A-C4A	7.32	1.52	1.39
4	A	400	NAD	C2N-N1N	7.18	1.42	1.35
6	F	500	NDP	C5A-C4A	7.11	1.51	1.39
4	A	400	NAD	C5A-C4A	6.94	1.51	1.39
4	D	400	NAD	C2N-N1N	6.12	1.41	1.35
4	H	400	NAD	C2N-N1N	6.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	500	NDP	C5A-C4A	6.03	1.49	1.39
4	A	400	NAD	O4D-C1D	5.62	1.48	1.40
4	B	400	NAD	C6N-N1N	5.20	1.47	1.35
4	G	400	NAD	C6N-N1N	5.16	1.47	1.35
4	H	400	NAD	C6N-N1N	4.83	1.46	1.35
4	D	400	NAD	C1B-N9A	4.81	1.59	1.46
4	D	400	NAD	C6N-N1N	4.69	1.46	1.35
4	B	400	NAD	O4D-C1D	4.68	1.47	1.40
4	B	400	NAD	C1B-N9A	4.67	1.59	1.46
4	H	400	NAD	PN-O5D	-4.50	1.41	1.59
6	I	500	NDP	C1B-N9A	4.49	1.58	1.46
4	G	400	NAD	C2N-C3N	4.47	1.46	1.39
4	D	400	NAD	O4D-C1D	4.43	1.46	1.40
6	C	500	NDP	C1B-N9A	4.36	1.58	1.46
4	A	400	NAD	C6N-N1N	4.34	1.45	1.35
4	B	400	NAD	C2N-C3N	4.29	1.45	1.39
4	B	400	NAD	O4B-C1B	4.27	1.51	1.42
4	H	400	NAD	C1B-N9A	4.22	1.58	1.46
4	G	400	NAD	C1B-N9A	4.22	1.58	1.46
6	F	500	NDP	C4N-C5N	-4.10	1.38	1.49
4	H	400	NAD	O4B-C1B	4.09	1.51	1.42
4	D	400	NAD	C4N-C3N	4.03	1.45	1.39
4	A	400	NAD	O4B-C1B	4.02	1.51	1.42
4	A	400	NAD	C1B-N9A	3.95	1.57	1.46
4	D	400	NAD	O4B-C1B	3.95	1.51	1.42
6	I	500	NDP	C4N-C5N	-3.89	1.38	1.49
4	A	400	NAD	C2N-C3N	3.79	1.45	1.39
4	D	400	NAD	PA-O3	3.74	1.63	1.59
6	F	500	NDP	C1B-N9A	3.74	1.56	1.46
4	G	400	NAD	O4B-C1B	3.71	1.50	1.42
6	I	500	NDP	C2N-C3N	3.69	1.45	1.35
6	F	500	NDP	C4N-C3N	-3.65	1.43	1.50
6	C	500	NDP	C4N-C5N	-3.65	1.39	1.49
4	D	400	NAD	C2N-C3N	3.60	1.44	1.39
6	F	500	NDP	C2N-C3N	3.58	1.45	1.35
4	G	400	NAD	C4N-C3N	3.52	1.44	1.39
4	B	400	NAD	C4N-C3N	3.51	1.44	1.39
4	H	400	NAD	C4N-C3N	3.51	1.44	1.39
4	D	400	NAD	C2A-N1A	3.43	1.40	1.33
6	F	500	NDP	C2D-C1D	3.41	1.64	1.53
4	H	400	NAD	C2N-C3N	3.40	1.44	1.39
6	I	500	NDP	O4B-C1B	3.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	500	NDP	C4N-C3N	-3.37	1.43	1.50
6	C	500	NDP	O4B-C1B	3.34	1.49	1.42
6	C	500	NDP	C4N-C3N	-3.28	1.43	1.50
6	C	500	NDP	C6N-N1N	3.24	1.45	1.37
4	B	400	NAD	PN-O2N	3.21	1.70	1.55
6	I	500	NDP	C6N-N1N	3.15	1.44	1.37
6	F	500	NDP	C3B-C4B	-3.15	1.45	1.53
6	C	500	NDP	C3B-C2B	-3.13	1.46	1.53
6	F	500	NDP	O4B-C1B	3.13	1.49	1.42
4	G	400	NAD	C2A-N1A	3.07	1.39	1.33
6	I	500	NDP	C3B-C2B	-3.06	1.46	1.53
6	C	500	NDP	C2N-C3N	3.03	1.43	1.35
6	C	500	NDP	P2B-O3X	-3.01	1.43	1.54
4	H	400	NAD	C2A-N1A	2.98	1.39	1.33
6	I	500	NDP	C2A-N1A	2.93	1.39	1.33
6	F	500	NDP	C6N-N1N	2.92	1.44	1.37
4	D	400	NAD	C3B-C4B	-2.89	1.45	1.53
4	B	400	NAD	C8A-N9A	2.82	1.42	1.37
4	B	400	NAD	C2A-N1A	2.81	1.38	1.33
6	C	500	NDP	O4D-C1D	2.79	1.48	1.42
4	A	400	NAD	PN-O5D	-2.76	1.48	1.59
4	A	400	NAD	C4N-C3N	2.75	1.43	1.39
4	B	400	NAD	C2D-C3D	2.73	1.60	1.53
4	A	400	NAD	C2A-N1A	2.72	1.38	1.33
4	A	400	NAD	PA-O3	2.72	1.62	1.59
4	A	400	NAD	C2D-C3D	2.71	1.60	1.53
4	B	400	NAD	PA-O3	-2.68	1.56	1.59
6	F	500	NDP	C2B-C1B	-2.65	1.46	1.53
6	I	500	NDP	P2B-O3X	-2.62	1.45	1.54
6	C	500	NDP	C3B-C4B	-2.62	1.46	1.53
6	F	500	NDP	C2A-N1A	2.60	1.38	1.33
6	F	500	NDP	C3B-C2B	-2.60	1.47	1.53
4	G	400	NAD	C3B-C4B	-2.59	1.46	1.53
4	G	400	NAD	O2B-C2B	-2.59	1.36	1.43
4	D	400	NAD	O2B-C2B	-2.56	1.36	1.43
6	F	500	NDP	P2B-O3X	-2.56	1.45	1.54
4	D	400	NAD	C5A-N7A	-2.54	1.34	1.39
6	C	500	NDP	C1D-N1N	2.50	1.53	1.46
4	A	400	NAD	PN-O2N	-2.48	1.43	1.55
4	G	400	NAD	C2B-C1B	-2.48	1.45	1.53
4	B	400	NAD	O5B-C5B	-2.45	1.35	1.44
6	I	500	NDP	C3B-C4B	-2.43	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	400	NAD	C2B-C3B	-2.43	1.46	1.53
6	I	500	NDP	P2B-O2X	-2.42	1.45	1.54
4	G	400	NAD	C2D-C3D	2.41	1.59	1.53
6	I	500	NDP	O2B-C2B	-2.41	1.35	1.44
4	G	400	NAD	C2B-C3B	-2.40	1.46	1.53
4	B	400	NAD	C2B-C3B	-2.39	1.46	1.53
4	H	400	NAD	C2B-C1B	-2.38	1.46	1.53
4	B	400	NAD	O2B-C2B	-2.36	1.37	1.43
6	C	500	NDP	C2B-C1B	-2.35	1.47	1.53
6	F	500	NDP	PA-O3	2.35	1.62	1.59
6	C	500	NDP	C2A-N1A	2.33	1.38	1.33
6	I	500	NDP	PA-O3	2.31	1.62	1.59
4	H	400	NAD	O2B-C2B	-2.31	1.37	1.43
6	I	500	NDP	C2B-C1B	-2.29	1.47	1.53
4	A	400	NAD	O2B-C2B	-2.27	1.37	1.43
6	C	500	NDP	O2B-C2B	-2.27	1.36	1.44
4	H	400	NAD	C2B-C3B	-2.27	1.47	1.53
4	A	400	NAD	PN-O1N	-2.23	1.43	1.50
6	F	500	NDP	P2B-O2X	-2.21	1.46	1.54
4	H	400	NAD	C3B-C4B	-2.20	1.47	1.53
4	B	400	NAD	C2B-C1B	-2.19	1.46	1.53
4	G	400	NAD	C8A-N9A	2.15	1.41	1.37
4	B	400	NAD	C5B-C4B	-2.15	1.45	1.51
4	A	400	NAD	O3B-C3B	2.13	1.48	1.43
4	H	400	NAD	O3D-C3D	2.13	1.48	1.43
4	A	400	NAD	C2B-C1B	-2.12	1.46	1.53
4	B	400	NAD	C3B-C4B	-2.11	1.47	1.53
4	B	400	NAD	C5D-C4D	-2.10	1.45	1.51
4	A	400	NAD	C8A-N9A	2.08	1.41	1.37
6	C	500	NDP	O3B-C3B	2.07	1.48	1.43
6	F	500	NDP	O2B-C2B	-2.04	1.37	1.44
4	H	400	NAD	C2D-C3D	2.03	1.58	1.53
6	C	500	NDP	P2B-O2X	-2.03	1.47	1.54
4	A	400	NAD	O3D-C3D	2.01	1.47	1.43

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	NAD	C4D-O4D-C1D	-11.28	99.60	109.92
4	G	400	NAD	O5D-C5D-C4D	9.92	142.78	108.99
4	G	400	NAD	C4D-O4D-C1D	-9.73	101.01	109.92
4	B	400	NAD	O4B-C4B-C5B	8.82	137.60	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	NAD	C6N-N1N-C2N	-8.76	114.42	121.88
4	H	400	NAD	C4D-O4D-C1D	-8.59	102.06	109.92
4	G	400	NAD	C6N-N1N-C2N	-8.06	115.02	121.88
6	C	500	NDP	P2B-O2B-C2B	7.91	144.55	123.43
4	A	400	NAD	C6N-N1N-C2N	-7.89	115.17	121.88
6	F	500	NDP	P2B-O2B-C2B	7.65	143.87	123.43
6	I	500	NDP	P2B-O2B-C2B	7.47	143.39	123.43
4	H	400	NAD	C6N-N1N-C2N	-7.28	115.68	121.88
4	D	400	NAD	C6N-N1N-C2N	-7.23	115.73	121.88
4	D	400	NAD	C4D-O4D-C1D	-6.40	104.06	109.92
4	A	400	NAD	C4D-O4D-C1D	-6.04	104.40	109.92
4	B	400	NAD	O5D-C5D-C4D	5.97	129.33	108.99
4	H	400	NAD	O4D-C4D-C3D	5.20	115.47	105.15
4	A	400	NAD	O2B-C2B-C3B	4.82	127.26	111.82
4	A	400	NAD	O4D-C4D-C3D	4.80	114.68	105.15
4	B	400	NAD	C2B-C3B-C4B	4.72	111.74	102.61
4	D	400	NAD	O4D-C4D-C3D	4.69	114.46	105.15
4	H	400	NAD	O2B-C2B-C3B	4.64	126.68	111.82
6	C	500	NDP	O5B-C5B-C4B	4.60	124.65	108.99
6	I	500	NDP	C2D-C1D-N1N	4.56	124.53	113.31
4	B	400	NAD	O2B-C2B-C3B	4.55	126.39	111.82
4	G	400	NAD	O4D-C4D-C3D	4.52	114.12	105.15
6	I	500	NDP	O5B-C5B-C4B	4.51	124.34	108.99
4	A	400	NAD	O5D-C5D-C4D	4.49	124.28	108.99
4	A	400	NAD	PN-O5D-C5D	4.47	146.98	121.35
6	F	500	NDP	C2B-C3B-C4B	4.45	111.55	101.99
6	C	500	NDP	O4D-C1D-N1N	-4.43	99.63	108.08
6	F	500	NDP	O5D-C5D-C4D	4.42	124.04	108.99
6	F	500	NDP	O5B-C5B-C4B	4.37	123.87	108.99
6	C	500	NDP	O5D-C5D-C4D	4.37	123.87	108.99
4	D	400	NAD	O5D-C5D-C4D	4.32	123.72	108.99
6	I	500	NDP	O4D-C4D-C3D	4.32	113.72	105.15
4	H	400	NAD	O5B-C5B-C4B	4.28	123.56	108.99
4	H	400	NAD	C2B-C3B-C4B	4.20	110.73	102.61
6	F	500	NDP	O4D-C4D-C3D	4.20	113.48	105.15
6	C	500	NDP	C6A-C5A-N7A	4.18	140.15	132.09
4	G	400	NAD	O2B-C2B-C3B	4.18	125.21	111.82
4	G	400	NAD	C2B-C3B-C4B	4.17	110.67	102.61
4	D	400	NAD	C4B-O4B-C1B	-4.16	100.28	109.47
6	C	500	NDP	C2B-C1B-N9A	4.13	120.55	113.75
4	A	400	NAD	C3N-C7N-N7N	-4.11	112.68	117.74
4	A	400	NAD	O5B-C5B-C4B	4.11	122.98	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	500	NDP	C6A-C5A-N7A	4.09	139.98	132.09
6	F	500	NDP	O2B-C2B-C3B	4.06	126.24	111.68
4	G	400	NAD	C3N-C7N-N7N	-4.06	112.74	117.74
4	A	400	NAD	C2B-C3B-C4B	4.05	110.44	102.61
4	G	400	NAD	O5B-C5B-C4B	4.02	122.68	108.99
6	I	500	NDP	C6A-C5A-N7A	3.95	139.70	132.09
6	C	500	NDP	C4A-N9A-C8A	3.91	109.85	105.74
6	C	500	NDP	C2B-C3B-C4B	3.90	110.39	101.99
4	H	400	NAD	C3N-C7N-N7N	-3.88	112.96	117.74
4	H	400	NAD	C6A-C5A-N7A	3.81	139.44	132.09
4	D	400	NAD	O2B-C2B-C3B	3.80	124.01	111.82
4	D	400	NAD	C2B-C3B-C4B	3.80	109.94	102.61
4	B	400	NAD	C6A-C5A-N7A	3.79	139.40	132.09
6	I	500	NDP	C4D-O4D-C1D	-3.79	101.11	109.47
6	F	500	NDP	C4A-N9A-C8A	3.78	109.71	105.74
4	D	400	NAD	O5B-C5B-C4B	3.78	121.86	108.99
6	C	500	NDP	C6A-C5A-C4A	-3.76	112.05	117.18
4	A	400	NAD	C6A-C5A-N7A	3.75	139.32	132.09
4	A	400	NAD	C4A-N9A-C8A	3.70	109.63	105.74
6	I	500	NDP	C6N-N1N-C2N	-3.66	115.40	119.32
4	D	400	NAD	O4B-C4B-C5B	3.66	121.04	109.33
4	G	400	NAD	PN-O5D-C5D	3.64	142.19	121.35
4	B	400	NAD	C6A-C5A-C4A	-3.63	112.22	117.18
4	B	400	NAD	C3N-C7N-N7N	-3.61	113.30	117.74
6	I	500	NDP	C4B-O4B-C1B	-3.60	101.51	109.47
6	I	500	NDP	O2B-C2B-C3B	3.60	124.59	111.68
4	A	400	NAD	N3A-C2A-N1A	-3.59	123.14	128.58
6	I	500	NDP	C2B-C3B-C4B	3.58	109.68	101.99
6	F	500	NDP	C6A-C5A-C4A	-3.56	112.31	117.18
4	B	400	NAD	N3A-C2A-N1A	-3.55	123.21	128.58
4	G	400	NAD	C4B-O4B-C1B	-3.52	101.70	109.47
6	C	500	NDP	O4D-C4D-C3D	3.49	112.09	105.15
4	B	400	NAD	O4D-C4D-C3D	3.49	112.08	105.15
6	F	500	NDP	O4D-C1D-N1N	-3.49	101.43	108.08
6	I	500	NDP	C2B-C1B-N9A	3.49	119.49	113.75
4	G	400	NAD	C6A-C5A-N7A	3.48	138.80	132.09
6	F	500	NDP	C6N-N1N-C2N	-3.48	115.60	119.32
6	I	500	NDP	PN-O5D-C5D	-3.47	101.46	121.35
4	H	400	NAD	N3A-C2A-N1A	-3.45	123.36	128.58
4	A	400	NAD	C6A-C5A-C4A	-3.45	112.47	117.18
4	G	400	NAD	C4A-N9A-C8A	3.44	109.35	105.74
6	C	500	NDP	N3A-C2A-N1A	-3.42	123.41	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	NAD	C4A-N9A-C8A	3.41	109.32	105.74
6	C	500	NDP	O2B-C2B-C3B	3.40	123.89	111.68
6	C	500	NDP	C4B-O4B-C1B	-3.37	102.02	109.47
4	G	400	NAD	C5N-C6N-N1N	3.37	124.97	120.38
6	C	500	NDP	C6N-N1N-C2N	-3.36	115.72	119.32
6	I	500	NDP	C5A-N7A-C8A	3.36	108.73	103.45
4	D	400	NAD	C6A-C5A-N7A	3.35	138.55	132.09
4	B	400	NAD	C5N-C6N-N1N	3.35	124.95	120.38
4	G	400	NAD	N3A-C2A-N1A	-3.35	123.51	128.58
6	I	500	NDP	C2D-C3D-C4D	-3.34	96.15	102.61
4	H	400	NAD	C6A-C5A-C4A	-3.34	112.62	117.18
4	A	400	NAD	C5N-C6N-N1N	3.34	124.94	120.38
6	C	500	NDP	C2D-C3D-C4D	-3.34	96.16	102.61
6	I	500	NDP	C6A-C5A-C4A	-3.33	112.63	117.18
4	D	400	NAD	C2B-C1B-N9A	3.32	121.56	113.30
6	C	500	NDP	C5A-N7A-C8A	3.31	108.65	103.45
4	H	400	NAD	C4A-N9A-C8A	3.29	109.20	105.74
4	A	400	NAD	C4B-O4B-C1B	-3.29	102.21	109.47
6	F	500	NDP	C5A-N7A-C8A	3.28	108.60	103.45
6	I	500	NDP	C4A-N9A-C8A	3.28	109.18	105.74
4	A	400	NAD	C5A-N7A-C8A	3.24	108.55	103.45
6	F	500	NDP	O2N-PN-O3	-3.24	98.51	107.27
4	D	400	NAD	C5A-N7A-C8A	3.21	108.50	103.45
6	F	500	NDP	C2B-C1B-N9A	3.21	119.03	113.75
4	D	400	NAD	O3D-C3D-C4D	3.20	120.29	111.08
4	G	400	NAD	C6A-C5A-C4A	-3.17	112.86	117.18
4	H	400	NAD	O3D-C3D-C4D	3.15	120.14	111.08
4	B	400	NAD	C5A-N7A-C8A	3.14	108.39	103.45
4	G	400	NAD	C5A-N7A-C8A	3.14	108.39	103.45
6	I	500	NDP	N3A-C2A-N1A	-3.13	123.84	128.58
4	H	400	NAD	C4B-O4B-C1B	-3.10	102.61	109.47
4	H	400	NAD	C6N-N1N-C1D	3.10	125.82	119.73
6	F	500	NDP	N3A-C2A-N1A	-3.06	123.96	128.58
4	H	400	NAD	O4B-C4B-C5B	3.05	119.12	109.33
6	I	500	NDP	C3N-C7N-N7N	-3.05	112.25	117.67
4	D	400	NAD	C3N-C7N-N7N	-3.04	114.00	117.74
4	D	400	NAD	C5N-C6N-N1N	3.03	124.52	120.38
6	I	500	NDP	O4B-C4B-C5B	3.02	119.00	109.33
4	H	400	NAD	C5A-N7A-C8A	3.01	108.19	103.45
6	F	500	NDP	O3D-C3D-C4D	3.01	119.73	111.08
4	A	400	NAD	O3-PN-O1N	3.01	119.75	110.70
4	H	400	NAD	C5N-C6N-N1N	3.00	124.48	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	400	NAD	C2B-C1B-N9A	3.00	120.76	113.30
4	G	400	NAD	O4B-C4B-C5B	2.99	118.91	109.33
4	A	400	NAD	O3D-C3D-C4D	2.93	119.51	111.08
4	A	400	NAD	C2D-C3D-C4D	-2.93	96.94	102.61
6	C	500	NDP	O4B-C4B-C5B	2.90	118.63	109.33
6	C	500	NDP	C2D-C1D-N1N	2.89	120.41	113.31
4	D	400	NAD	C4A-N9A-C8A	2.89	108.77	105.74
4	G	400	NAD	O3D-C3D-C4D	2.87	119.31	111.08
4	G	400	NAD	C5D-C4D-C3D	-2.84	104.98	115.21
4	D	400	NAD	N3A-C2A-N1A	-2.84	124.29	128.58
4	D	400	NAD	C6A-C5A-C4A	-2.84	113.30	117.18
6	C	500	NDP	O2N-PN-O3	-2.82	99.65	107.27
4	D	400	NAD	O2N-PN-O3	-2.78	99.75	107.27
4	G	400	NAD	C5A-C4A-N9A	-2.77	102.79	105.81
4	H	400	NAD	C5A-C4A-N9A	-2.73	102.84	105.81
4	G	400	NAD	C6N-N1N-C1D	2.71	125.05	119.73
4	B	400	NAD	O3D-C3D-C4D	2.70	118.84	111.08
6	I	500	NDP	O3D-C3D-C4D	2.70	118.83	111.08
6	C	500	NDP	O4B-C1B-N9A	-2.69	102.92	108.09
6	F	500	NDP	O4B-C4B-C5B	2.65	117.83	109.33
6	C	500	NDP	O5D-PN-O1N	2.64	119.42	108.94
4	A	400	NAD	C2N-C3N-C4N	2.64	121.32	118.26
6	C	500	NDP	C4D-O4D-C1D	-2.63	103.66	109.47
6	C	500	NDP	O4D-C4D-C5D	2.62	117.74	109.33
4	D	400	NAD	C5A-C4A-N9A	-2.61	102.96	105.81
4	A	400	NAD	O4B-C4B-C5B	2.60	117.68	109.33
6	C	500	NDP	N9A-C8A-N7A	-2.56	110.30	113.94
6	I	500	NDP	C4A-C5A-N7A	-2.55	107.67	110.58
4	A	400	NAD	C5A-C4A-N9A	-2.54	103.04	105.81
6	F	500	NDP	O5D-PN-O1N	2.54	119.02	108.94
6	F	500	NDP	C4D-O4D-C1D	-2.52	103.89	109.47
6	F	500	NDP	C4A-C5A-N7A	-2.52	107.70	110.58
4	A	400	NAD	PA-O5B-C5B	2.51	135.73	121.35
4	G	400	NAD	O4B-C1B-N9A	-2.51	103.28	108.09
4	B	400	NAD	C5A-C4A-N9A	-2.48	103.11	105.81
4	A	400	NAD	C2B-C1B-N9A	2.47	119.44	113.30
6	C	500	NDP	O3D-C3D-C4D	2.46	118.15	111.08
6	F	500	NDP	C3N-C7N-N7N	-2.45	113.31	117.67
4	B	400	NAD	O5D-PN-O1N	2.43	118.58	108.94
4	A	400	NAD	O2D-C2D-C3D	2.43	119.61	111.82
6	C	500	NDP	C4A-C5A-N7A	-2.43	107.81	110.58
6	F	500	NDP	C4B-O4B-C1B	-2.41	104.14	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	500	NDP	O3-PN-O1N	2.41	117.94	110.70
4	H	400	NAD	N3A-C4A-N9A	2.40	131.26	127.17
4	H	400	NAD	C2N-C3N-C4N	2.40	121.04	118.26
6	F	500	NDP	C3N-C2N-N1N	-2.39	119.70	123.20
6	F	500	NDP	N9A-C8A-N7A	-2.38	110.56	113.94
4	G	400	NAD	O2N-PN-O3	-2.37	100.87	107.27
4	A	400	NAD	N9A-C8A-N7A	-2.37	110.58	113.94
4	A	400	NAD	O7N-C7N-N7N	2.36	126.03	122.62
4	B	400	NAD	PN-O5D-C5D	2.35	134.82	121.35
4	H	400	NAD	PA-O5B-C5B	2.35	134.79	121.35
6	C	500	NDP	C2A-N1A-C6A	2.34	122.57	118.73
6	C	500	NDP	PN-O5D-C5D	2.33	134.68	121.35
4	B	400	NAD	C2A-N1A-C6A	2.32	122.55	118.73
4	G	400	NAD	O4D-C4D-C5D	-2.31	101.93	109.33
4	H	400	NAD	C4A-C5A-N7A	-2.31	107.94	110.58
4	G	400	NAD	N3A-C4A-N9A	2.31	131.09	127.17
4	H	400	NAD	C2A-N1A-C6A	2.30	122.51	118.73
4	A	400	NAD	O4D-C4D-C5D	2.30	116.70	109.33
4	A	400	NAD	O4B-C4B-C3B	-2.29	100.61	105.15
4	D	400	NAD	O4B-C1B-N9A	-2.29	103.69	108.09
4	B	400	NAD	C2N-C3N-C4N	2.29	120.92	118.26
6	F	500	NDP	C2D-C3D-C4D	-2.28	98.21	102.61
4	D	400	NAD	N3A-C4A-N9A	2.27	131.03	127.17
6	I	500	NDP	O2D-C2D-C3D	2.27	119.09	111.82
4	H	400	NAD	O5D-C5D-C4D	2.26	116.67	108.99
4	H	400	NAD	O7N-C7N-N7N	2.25	125.87	122.62
4	D	400	NAD	O4D-C4D-C5D	2.25	116.54	109.33
4	G	400	NAD	O4B-C4B-C3B	-2.24	100.70	105.15
4	D	400	NAD	O4B-C4B-C3B	-2.24	100.71	105.15
4	D	400	NAD	O5D-PN-O1N	2.24	117.80	108.94
4	B	400	NAD	N3A-C4A-N9A	2.24	130.97	127.17
6	F	500	NDP	PN-O5D-C5D	2.23	134.14	121.35
6	I	500	NDP	C3D-C2D-C1D	2.22	105.66	101.46
6	C	500	NDP	C5A-C4A-N9A	-2.22	103.39	105.81
4	A	400	NAD	C2A-N1A-C6A	2.21	122.37	118.73
6	F	500	NDP	O4B-C1B-N9A	-2.21	103.84	108.09
6	I	500	NDP	O4D-C1D-N1N	-2.21	103.87	108.08
4	B	400	NAD	N9A-C8A-N7A	-2.21	110.80	113.94
6	F	500	NDP	C2A-N1A-C6A	2.20	122.35	118.73
6	F	500	NDP	O4D-C4D-C5D	2.19	116.36	109.33
4	D	400	NAD	C2D-C3D-C4D	-2.18	98.39	102.61
6	F	500	NDP	C5A-C4A-N9A	-2.18	103.43	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	500	NDP	O4B-C4B-C3B	-2.18	100.82	105.15
4	A	400	NAD	N3A-C4A-N9A	2.17	130.87	127.17
4	H	400	NAD	O4B-C4B-C3B	-2.15	100.88	105.15
4	G	400	NAD	C2N-C3N-C4N	2.15	120.76	118.26
6	I	500	NDP	N9A-C8A-N7A	-2.14	110.90	113.94
4	D	400	NAD	C4A-C5A-N7A	-2.13	108.14	110.58
4	G	400	NAD	PA-O5B-C5B	2.13	133.54	121.35
4	G	400	NAD	C2A-N1A-C6A	2.12	122.22	118.73
6	C	500	NDP	O2D-C2D-C3D	2.11	118.59	111.82
4	D	400	NAD	PN-O5D-C5D	2.11	133.43	121.35
6	I	500	NDP	N3A-C4A-N9A	2.11	130.75	127.17
6	I	500	NDP	C5A-C4A-N9A	-2.11	103.52	105.81
6	C	500	NDP	O2A-PA-O1A	2.11	122.24	112.44
6	C	500	NDP	O4B-C4B-C3B	-2.10	100.98	105.15
4	B	400	NAD	C2D-C3D-C4D	-2.10	98.55	102.61
4	G	400	NAD	O2D-C2D-C3D	2.09	118.51	111.82
4	A	400	NAD	C4A-C5A-N7A	-2.08	108.21	110.58
6	I	500	NDP	C3N-C2N-N1N	-2.06	120.19	123.20
6	I	500	NDP	O2A-PA-O1A	2.05	121.98	112.44
6	I	500	NDP	PA-O5B-C5B	2.04	133.05	121.35
4	D	400	NAD	C2N-C3N-C4N	2.03	120.62	118.26
4	B	400	NAD	O2N-PN-O1N	2.02	121.86	112.44
4	A	400	NAD	O4B-C1B-N9A	-2.01	104.23	108.09
6	F	500	NDP	N3A-C4A-N9A	2.00	130.58	127.17
4	D	400	NAD	C2A-N1A-C6A	2.00	122.02	118.73

There are no chirality outliers.

All (99) 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-O3
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	C2D-C1D-N1N-C2N
4	B	400	NAD	C2D-C1D-N1N-C6N
4	B	400	NAD	C2N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
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-O3
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	G	400	NAD	C5B-O5B-PA-O3
4	H	400	NAD	C5B-O5B-PA-O1A
4	H	400	NAD	C5B-O5B-PA-O2A
4	H	400	NAD	C5B-O5B-PA-O3
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	C2N-C3N-C7N-N7N
6	F	500	NDP	C5B-O5B-PA-O1A
6	F	500	NDP	C5D-O5D-PN-O2N
6	F	500	NDP	C2N-C3N-C7N-N7N
6	I	500	NDP	C5B-O5B-PA-O2A
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	H	400	NAD	O4D-C4D-C5D-O5D
6	F	500	NDP	O4B-C4B-C5B-O5B
6	F	500	NDP	C1B-C2B-O2B-P2B
6	I	500	NDP	C1B-C2B-O2B-P2B
4	A	400	NAD	C2N-C3N-C7N-O7N
4	B	400	NAD	O4B-C4B-C5B-O5B
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	I	500	NDP	O4B-C4B-C5B-O5B
4	A	400	NAD	C2N-C3N-C7N-N7N
6	C	500	NDP	C2D-C1D-N1N-C6N
6	F	500	NDP	C2D-C1D-N1N-C6N
6	C	500	NDP	C3B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
6	F	500	NDP	C3B-C2B-O2B-P2B
6	I	500	NDP	C3B-C2B-O2B-P2B
4	B	400	NAD	O4D-C4D-C5D-O5D
4	D	400	NAD	C3D-C4D-C5D-O5D
4	H	400	NAD	C3D-C4D-C5D-O5D
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	C	500	NDP	O4D-C4D-C5D-O5D
6	F	500	NDP	O4D-C4D-C5D-O5D
6	I	500	NDP	C3B-C4B-C5B-O5B
4	A	400	NAD	C4N-C3N-C7N-O7N
4	A	400	NAD	C4N-C3N-C7N-N7N
4	A	400	NAD	C4D-C5D-O5D-PN
4	H	400	NAD	C4B-C5B-O5B-PA
6	C	500	NDP	C3B-C4B-C5B-O5B
4	B	400	NAD	C2B-C1B-N9A-C4A
4	G	400	NAD	C4D-C5D-O5D-PN
4	B	400	NAD	PN-O3-PA-O5B
6	C	500	NDP	O4D-C1D-N1N-C2N
6	C	500	NDP	O4D-C1D-N1N-C6N
4	B	400	NAD	C4D-C5D-O5D-PN
4	B	400	NAD	C2B-C1B-N9A-C8A
4	H	400	NAD	O4B-C4B-C5B-O5B
4	G	400	NAD	O4D-C4D-C5D-O5D
6	I	500	NDP	C5B-O5B-PA-O1A
6	I	500	NDP	C5B-O5B-PA-O3
4	G	400	NAD	C4B-C5B-O5B-PA
6	F	500	NDP	O4D-C1D-N1N-C2N
6	F	500	NDP	O4D-C1D-N1N-C6N
4	H	400	NAD	O4B-C1B-N9A-C8A
4	H	400	NAD	O4B-C1B-N9A-C4A
4	D	400	NAD	O4D-C1D-N1N-C2N
6	I	500	NDP	O4D-C1D-N1N-C6N
4	B	400	NAD	PN-O3-PA-O1A
4	A	400	NAD	O4D-C4D-C5D-O5D
4	D	400	NAD	O4B-C4B-C5B-O5B
6	I	500	NDP	C2D-C1D-N1N-C6N
4	G	400	NAD	O4B-C1B-N9A-C4A
4	G	400	NAD	O4B-C1B-N9A-C8A
4	B	400	NAD	PA-O3-PN-O1N
4	G	400	NAD	C3D-C4D-C5D-O5D

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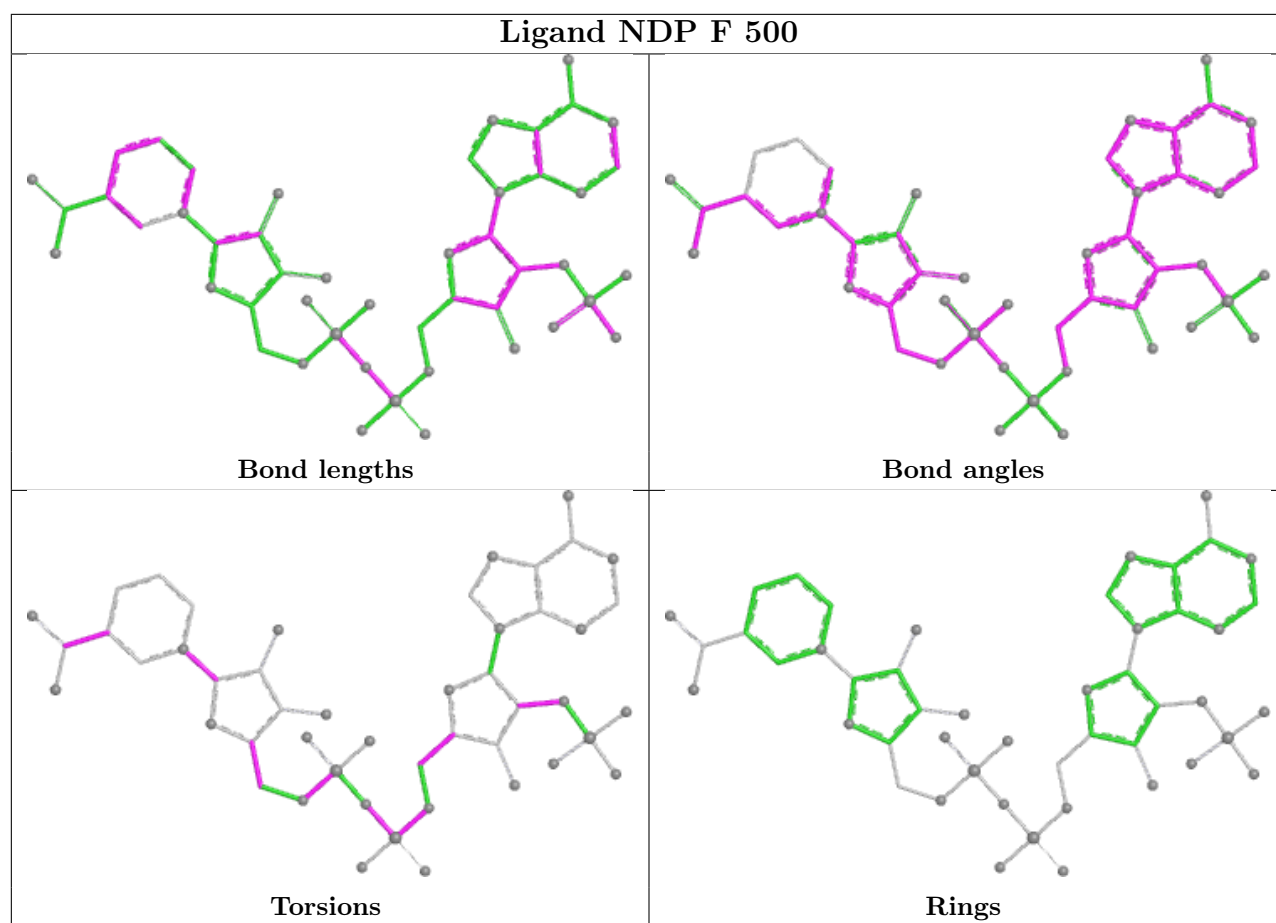
Mol	Chain	Res	Type	Atoms
6	C	500	NDP	C3D-C4D-C5D-O5D
6	C	500	NDP	PN-O3-PA-O2A
6	F	500	NDP	PN-O3-PA-O2A

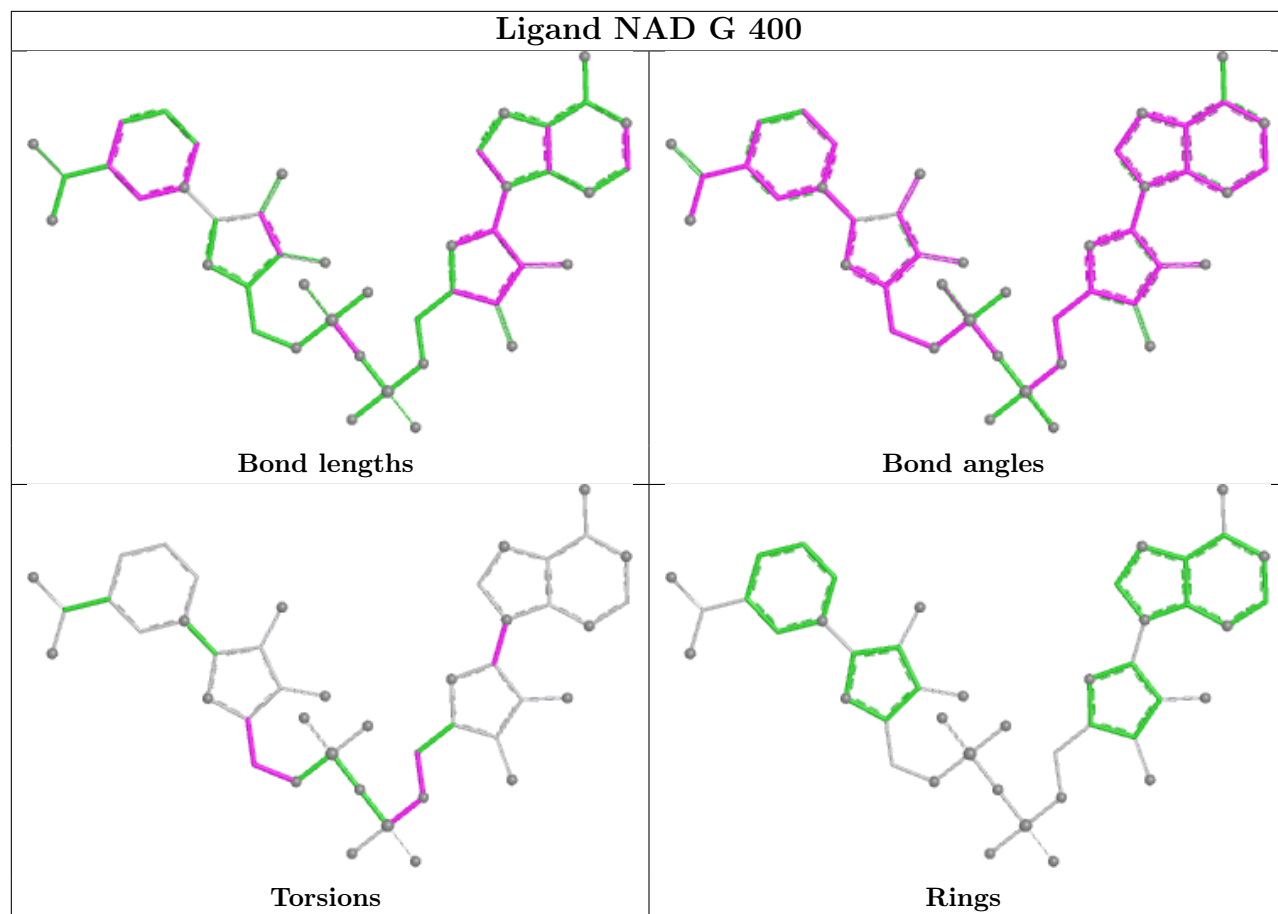
There are no ring outliers.

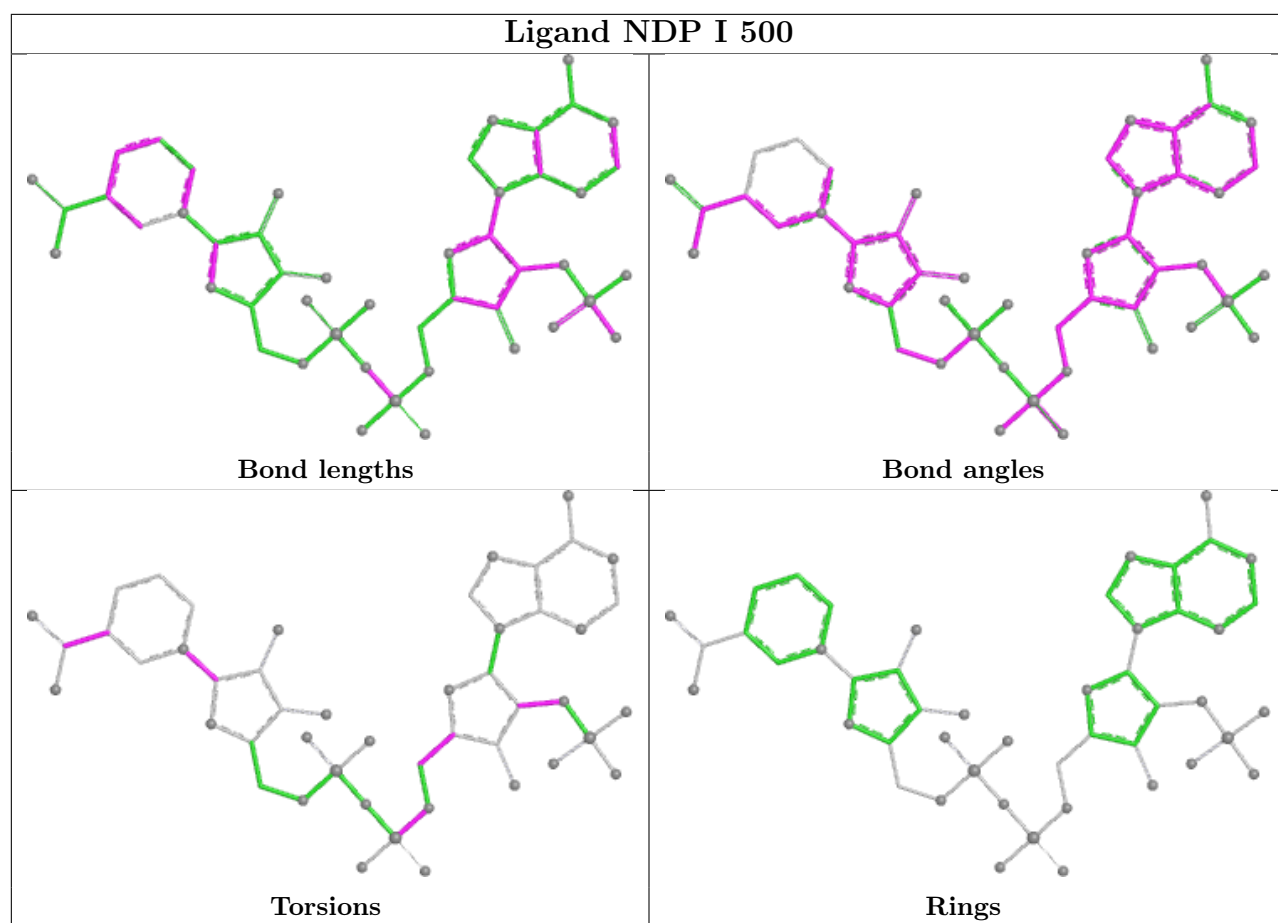
8 monomers are involved in 46 short contacts:

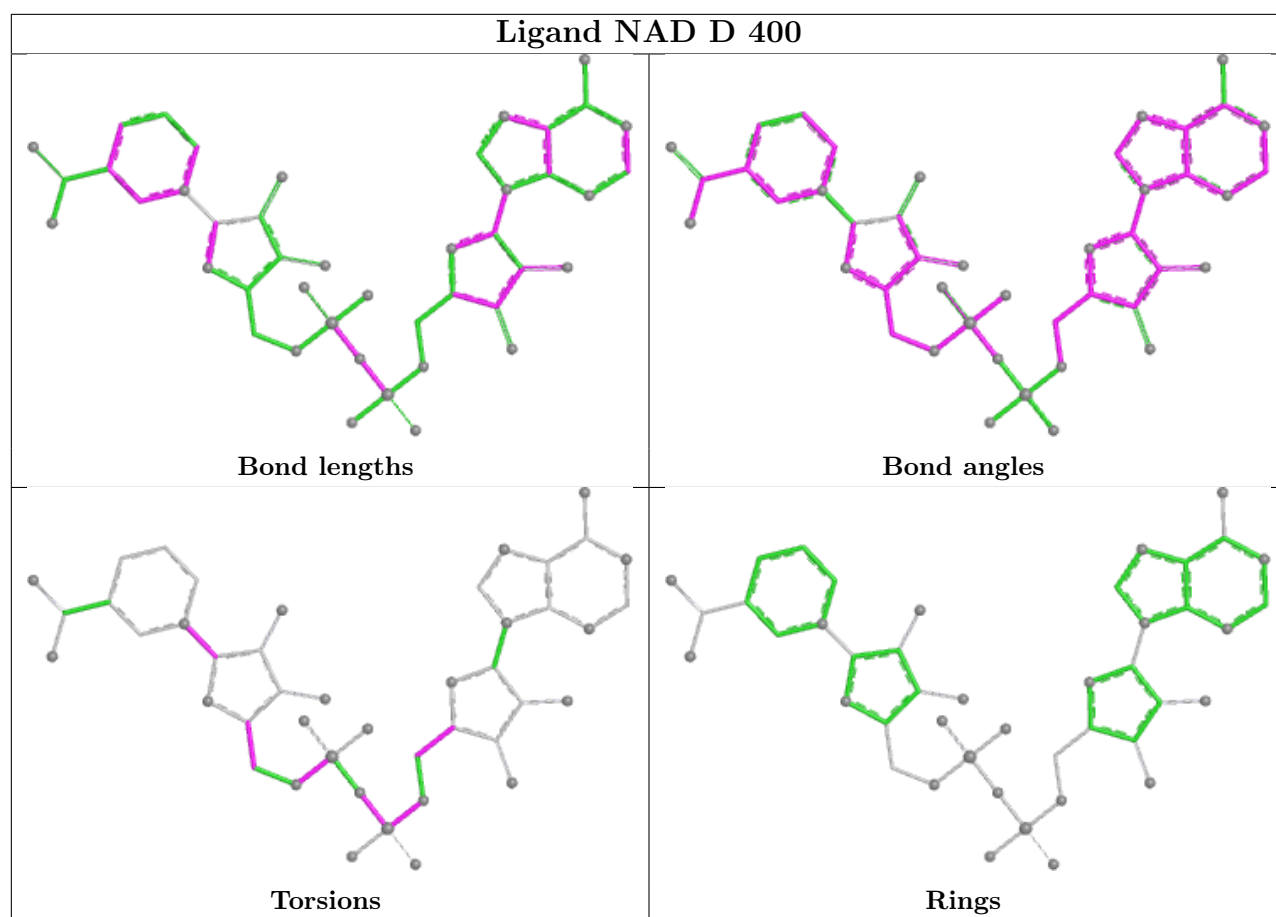
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	500	NDP	10	0
4	G	400	NAD	6	0
6	I	500	NDP	3	0
4	D	400	NAD	3	0
4	B	400	NAD	9	0
4	H	400	NAD	8	0
4	A	400	NAD	2	0
6	C	500	NDP	5	0

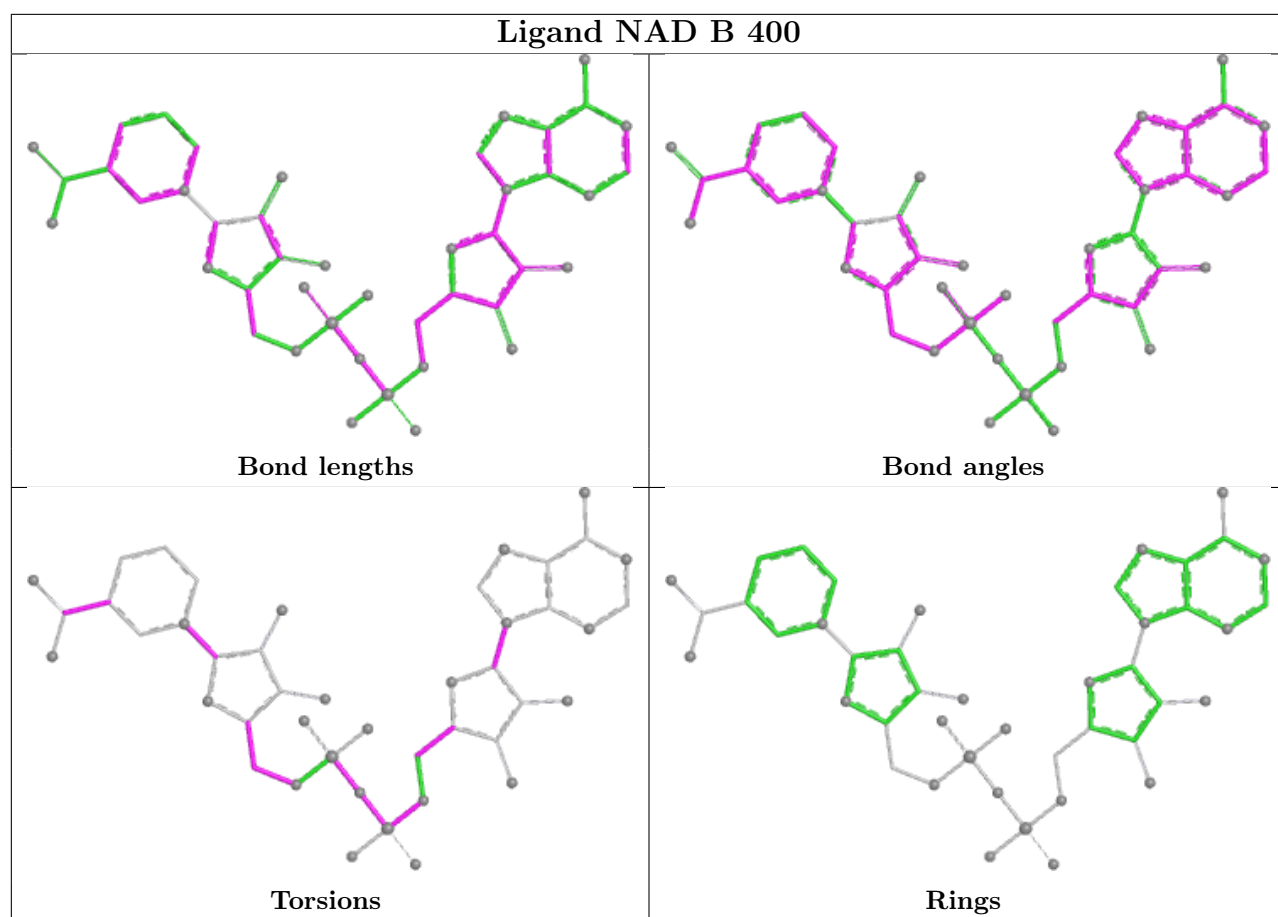
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

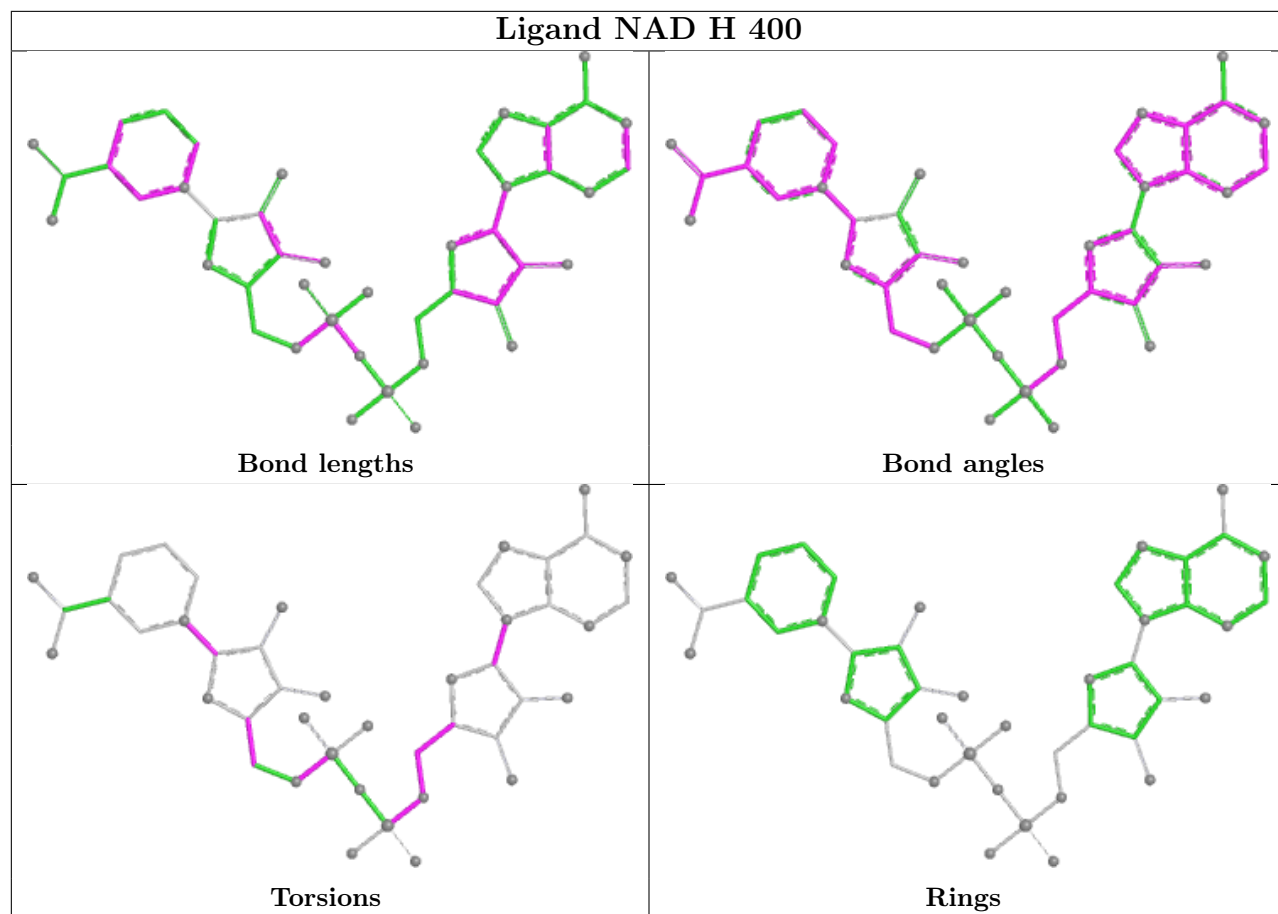


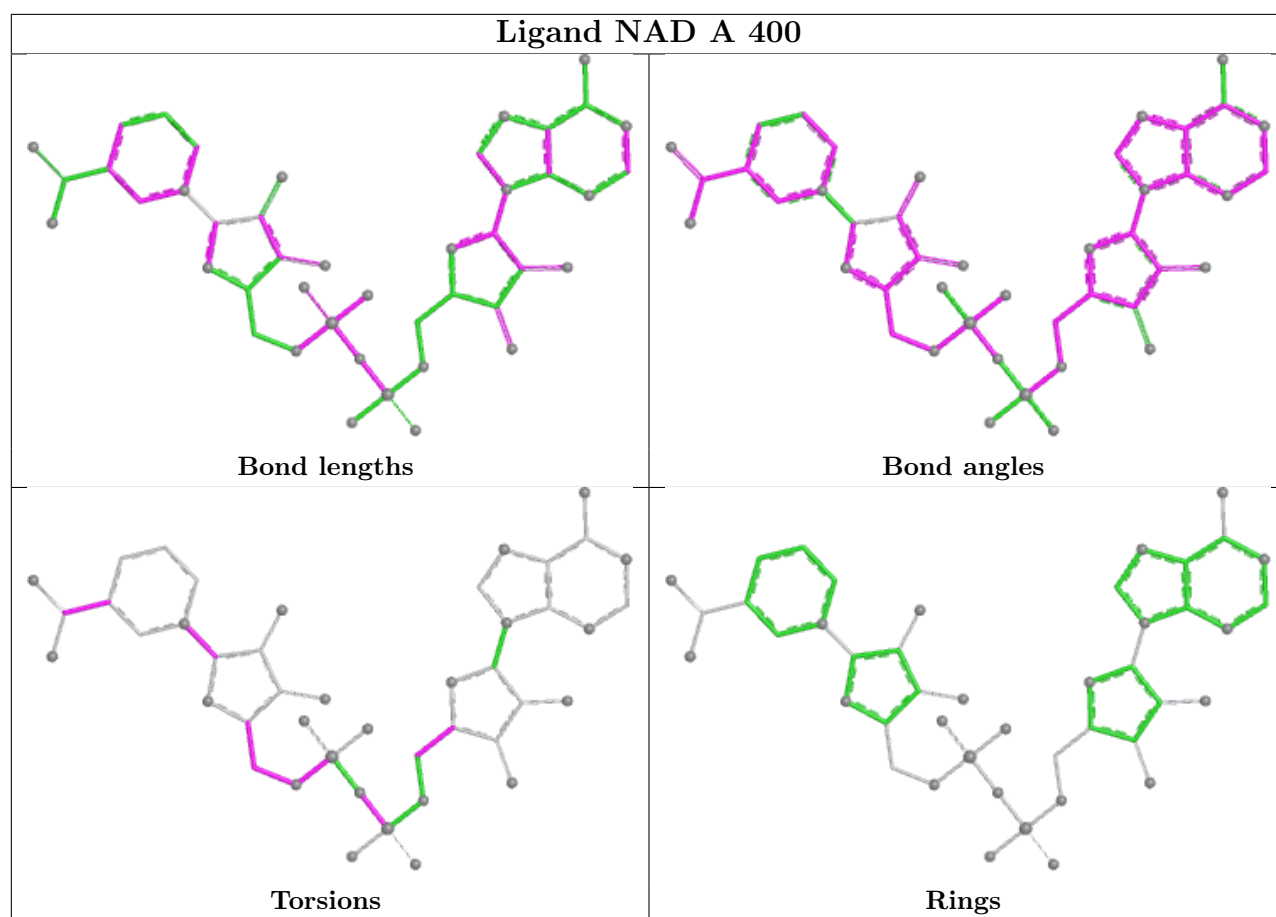


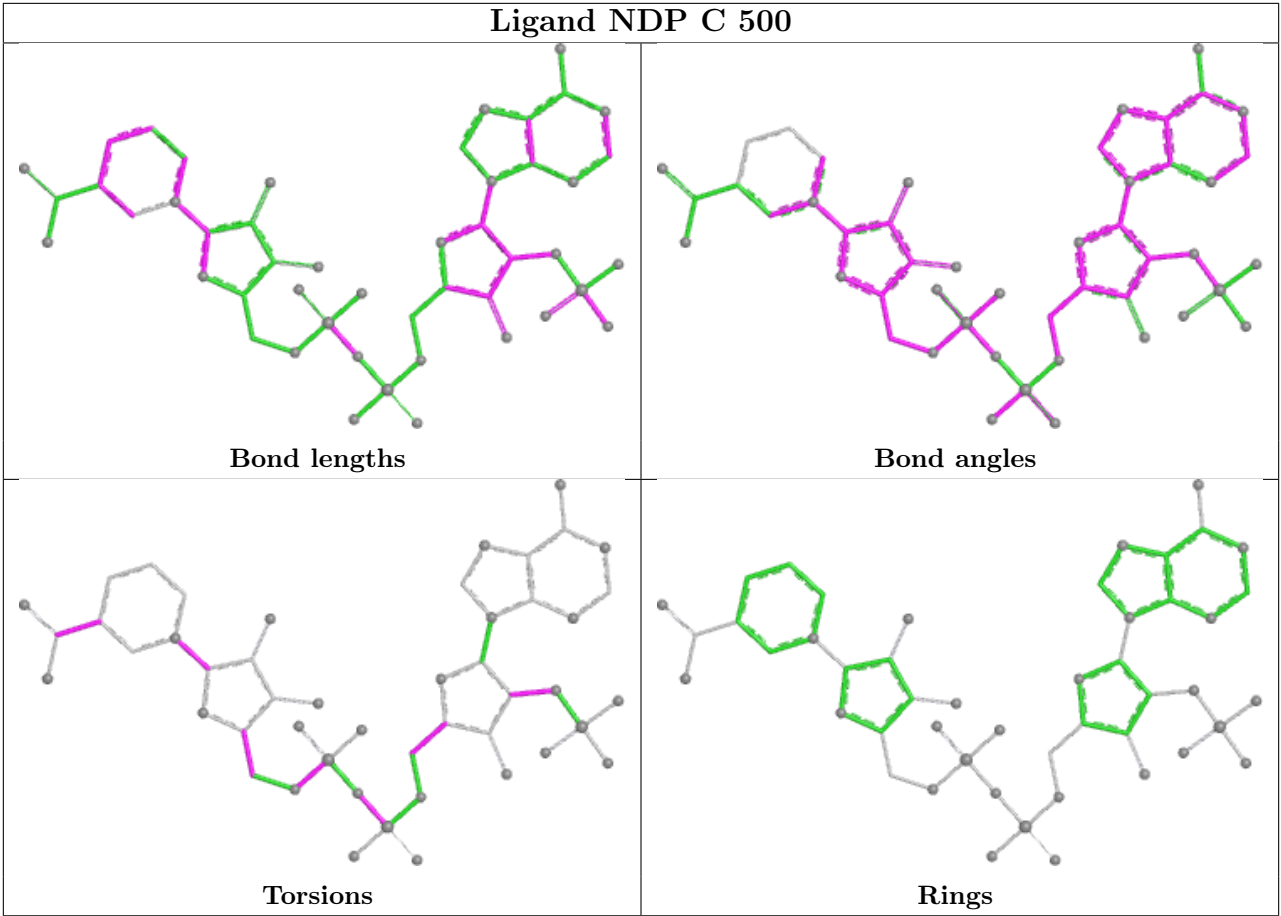












5.7 Other polymers ⓘ

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/384 (94%)	-0.42	0 100 100	30, 51, 77, 102	0
1	B	359/384 (93%)	-0.42	0 100 100	28, 52, 72, 98	0
1	D	378/384 (98%)	-0.05	4 (1%) 78 59	36, 68, 94, 104	0
1	E	359/384 (93%)	-0.37	1 (0%) 90 80	33, 60, 79, 91	0
1	G	364/384 (94%)	-0.31	0 100 100	35, 59, 84, 102	0
1	H	357/384 (92%)	-0.02	3 (0%) 82 65	39, 72, 96, 104	0
2	C	174/174 (100%)	-0.50	0 100 100	32, 47, 61, 68	0
2	F	173/174 (99%)	-0.40	0 100 100	40, 52, 63, 75	0
2	I	173/174 (99%)	-0.31	0 100 100	42, 58, 73, 79	0
All	All	2700/2826 (95%)	-0.29	8 (0%) 90 80	28, 57, 90, 104	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	371	ASP	2.9
1	D	225	ALA	2.8
1	E	378	ALA	2.6
1	H	267	ILE	2.5
1	H	64	ALA	2.5
1	D	221	VAL	2.4
1	D	224	GLU	2.3
1	H	202	ASP	2.3

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

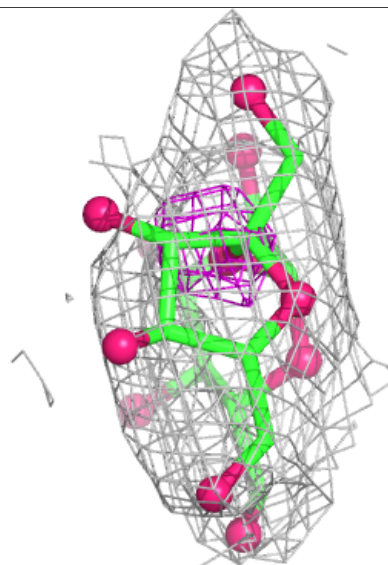
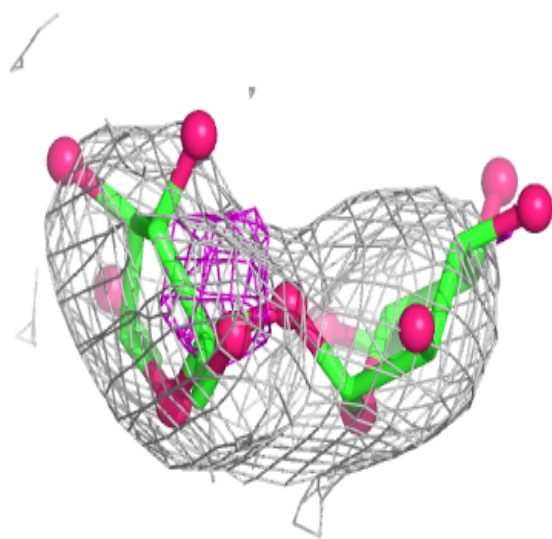
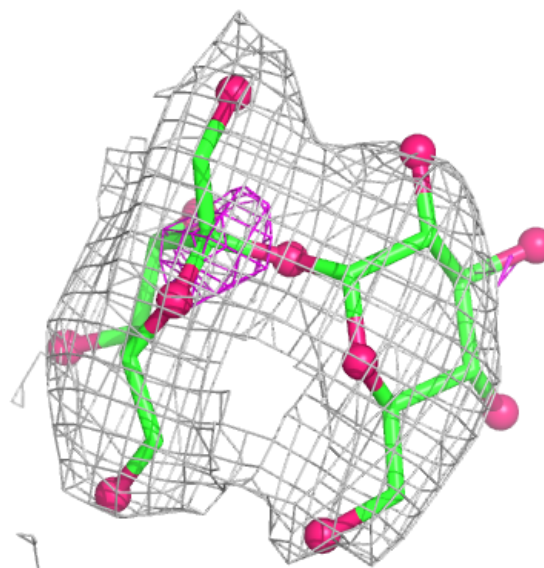
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FRU	N	2	12/12	0.47	0.15	98,99,99,99	0
3	GLC	O	1	11/12	0.60	0.11	82,83,83,84	0
3	GLC	J	1	11/12	0.63	0.11	76,77,79,79	0
3	GLC	N	1	11/12	0.65	0.16	97,99,99,99	0
3	FRU	K	2	12/12	0.67	0.15	84,88,89,89	0
3	FRU	L	2	12/12	0.69	0.14	81,82,83,83	0
3	GLC	M	1	11/12	0.74	0.09	76,76,77,77	0
3	GLC	L	1	11/12	0.77	0.10	79,82,82,83	0
3	FRU	O	2	12/12	0.79	0.13	84,85,85,87	0
3	GLC	K	1	11/12	0.81	0.08	86,88,88,88	0
3	FRU	J	2	12/12	0.82	0.12	70,73,75,76	0
3	FRU	M	2	12/12	0.84	0.12	70,74,75,76	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.

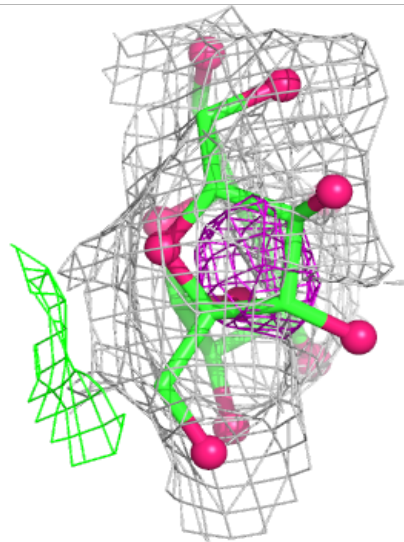
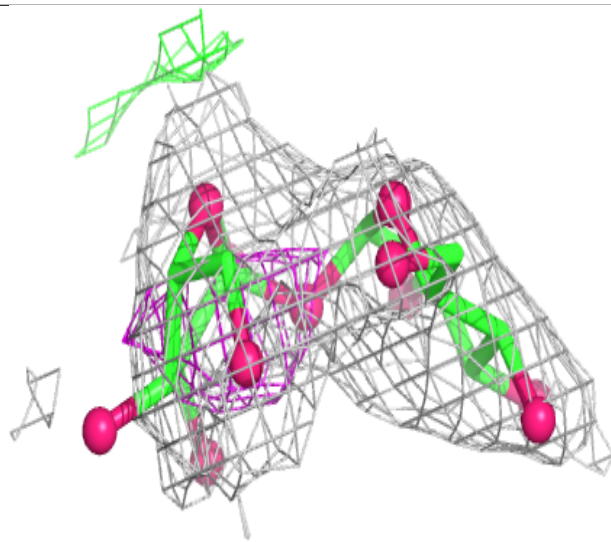
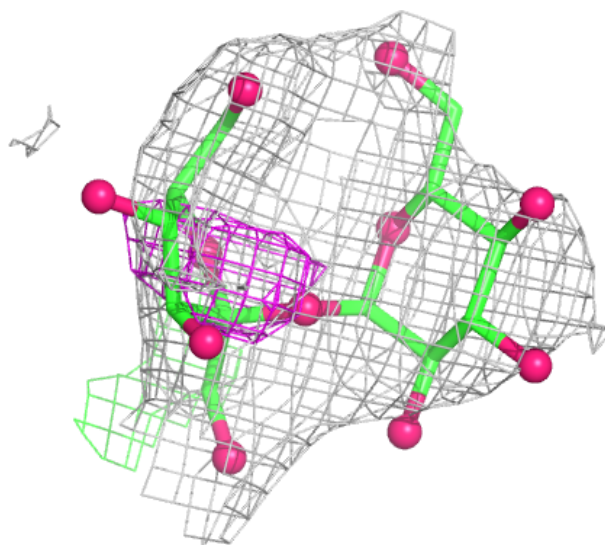
Electron density around Chain J:

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



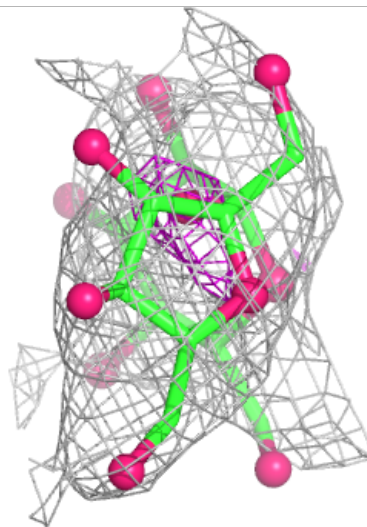
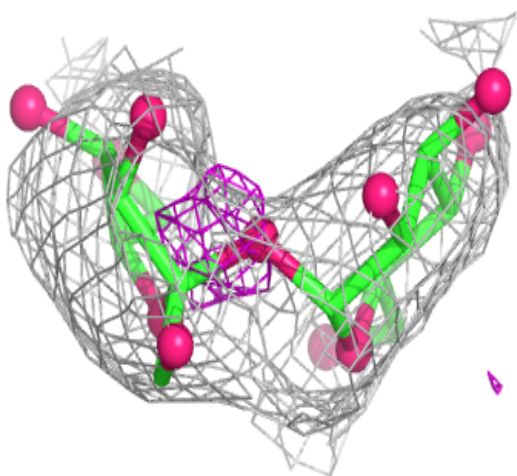
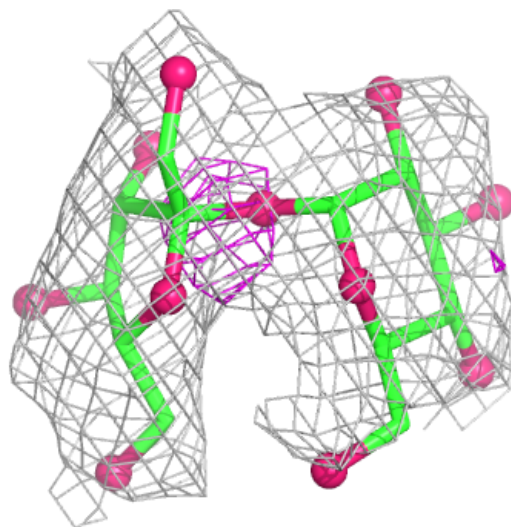
Electron density around Chain K:

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



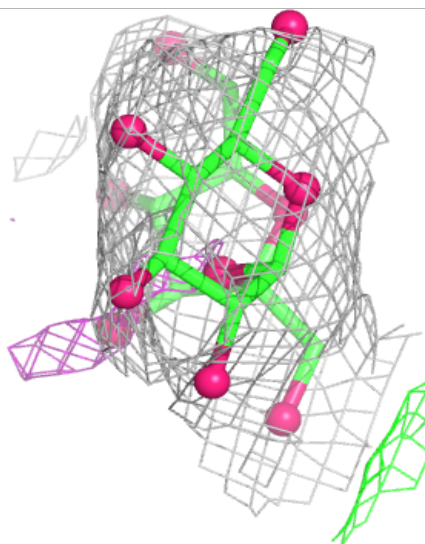
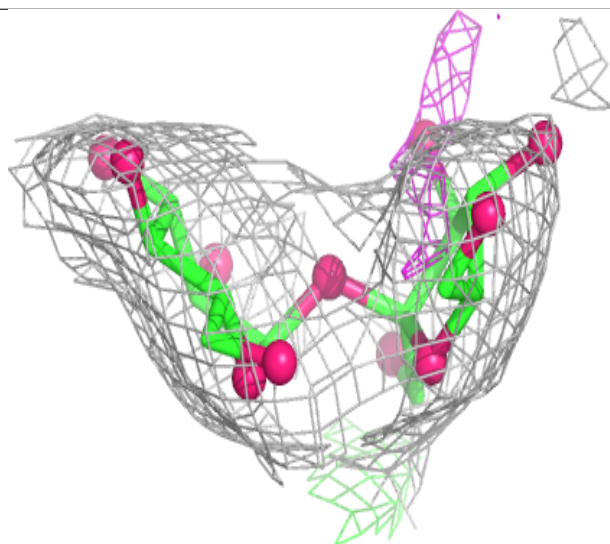
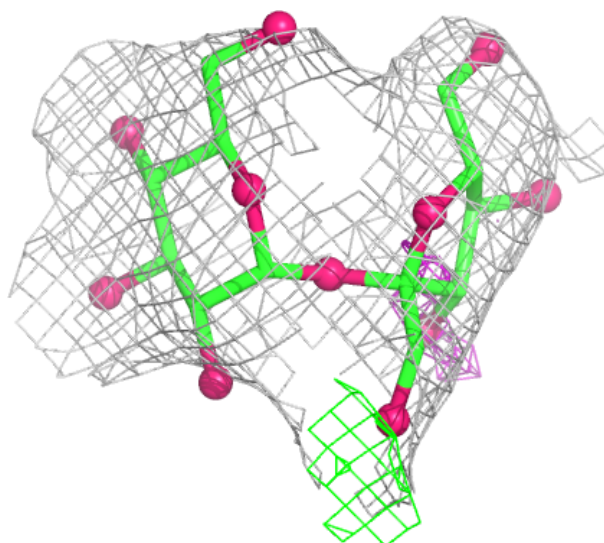
Electron density around Chain L:

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



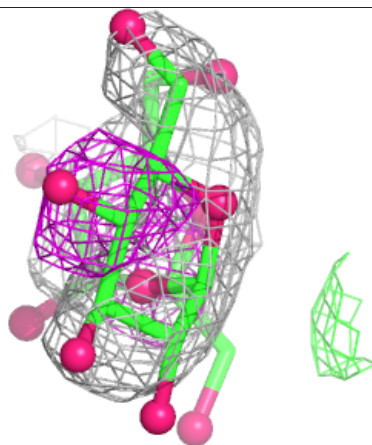
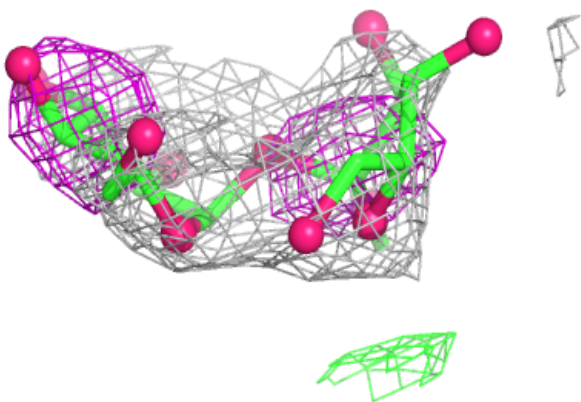
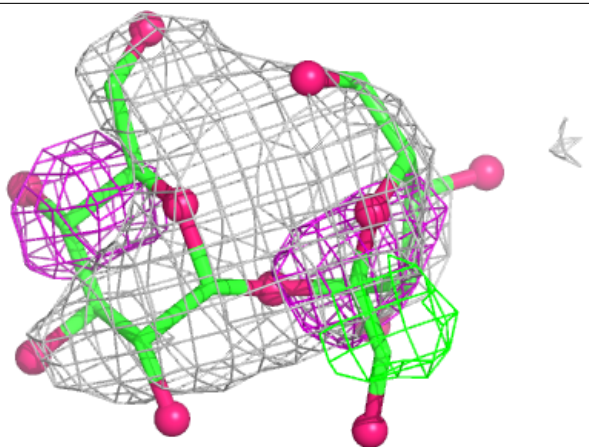
Electron density around Chain M:

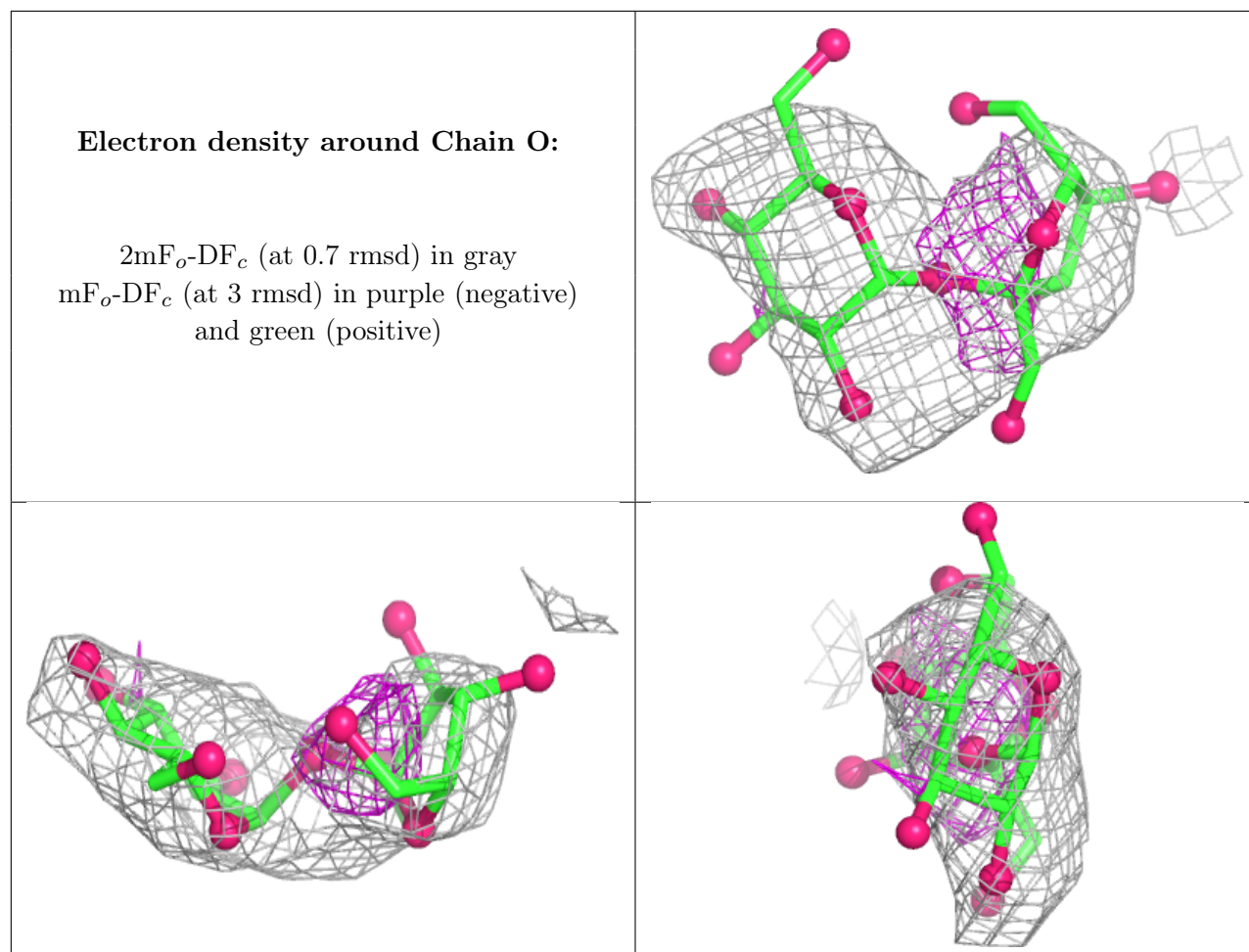
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)



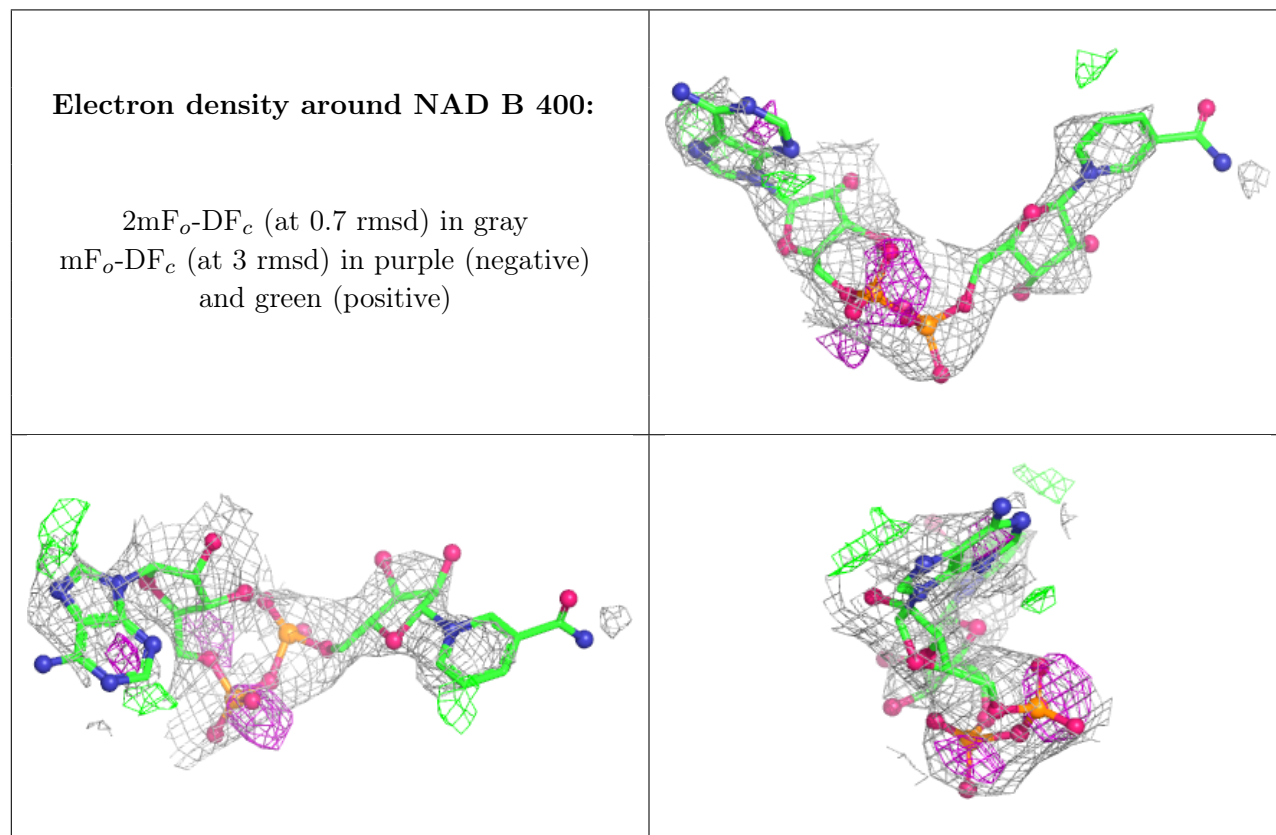


6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

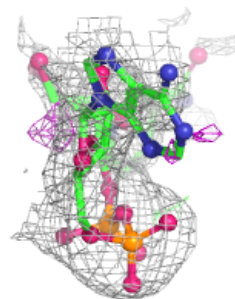
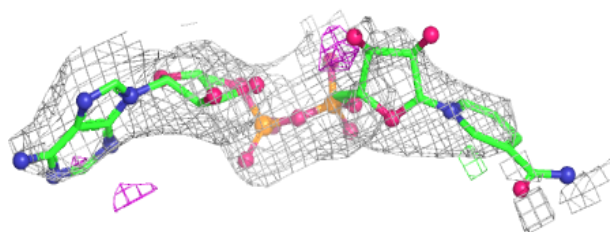
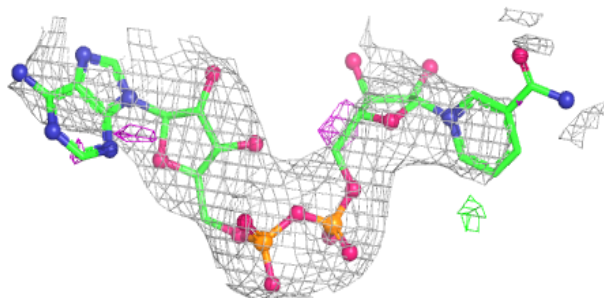
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAD	B	400	44/44	0.66	0.14	104,104,105,105	0
4	NAD	H	400	44/44	0.81	0.12	88,90,99,101	0
4	NAD	G	400	44/44	0.84	0.12	65,72,87,87	0
4	NAD	D	400	44/44	0.89	0.11	54,60,64,65	0
5	NA	D	602	1/1	0.91	0.10	69,69,69,69	0
4	NAD	A	400	44/44	0.92	0.09	65,71,75,75	0
6	NDP	I	500	48/48	0.92	0.08	56,58,64,64	0
5	NA	G	603	1/1	0.95	0.12	48,48,48,48	0
6	NDP	F	500	48/48	0.95	0.07	48,52,56,58	0
5	NA	A	601	1/1	0.95	0.05	50,50,50,50	0
6	NDP	C	500	48/48	0.97	0.06	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.

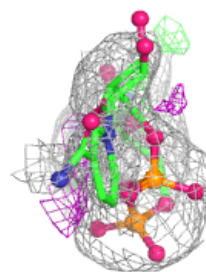
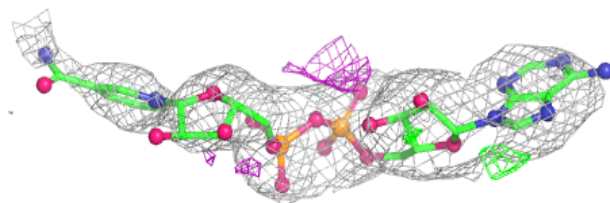
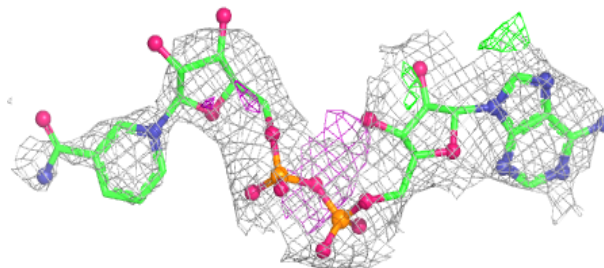


Electron density around NAD H 400:

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

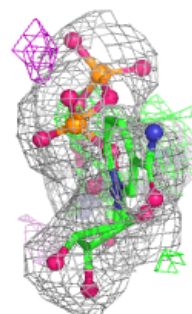
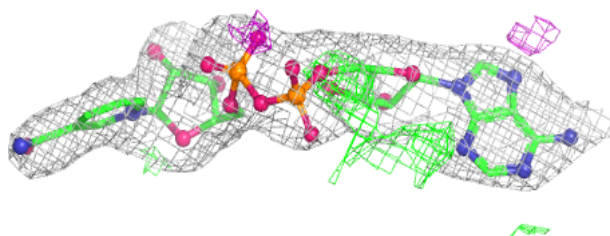
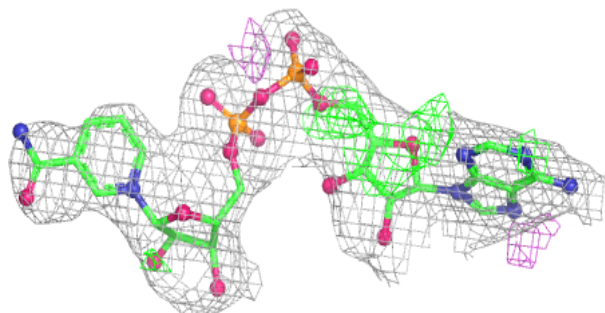
**Electron density around NAD G 400:**

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

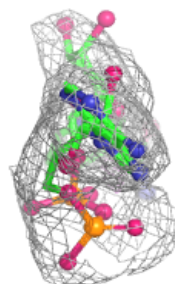
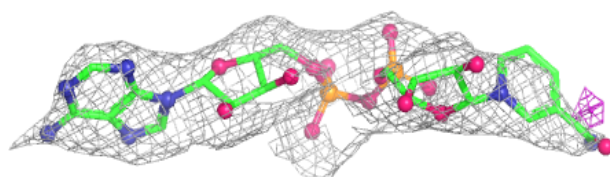
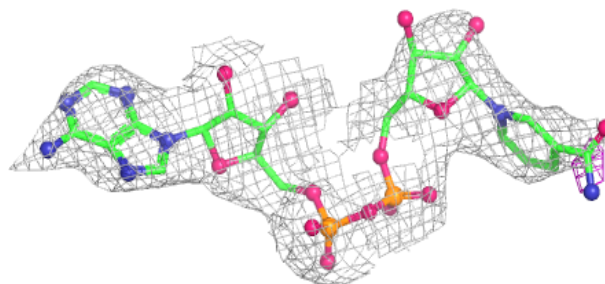


Electron density around NAD D 400:

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

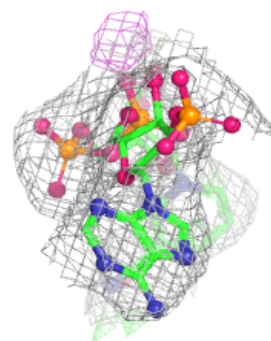
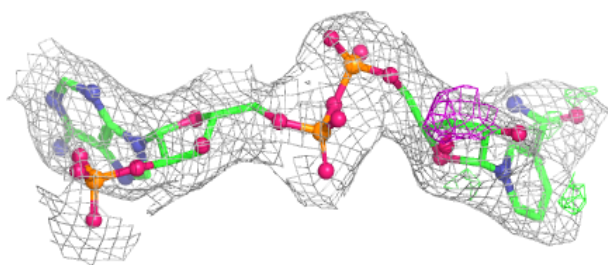
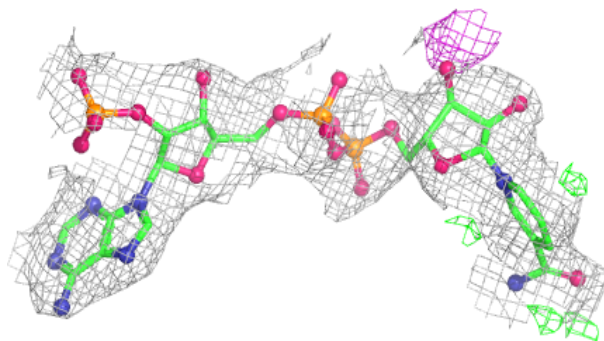
**Electron density around NAD A 400:**

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

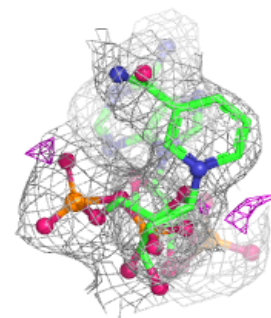
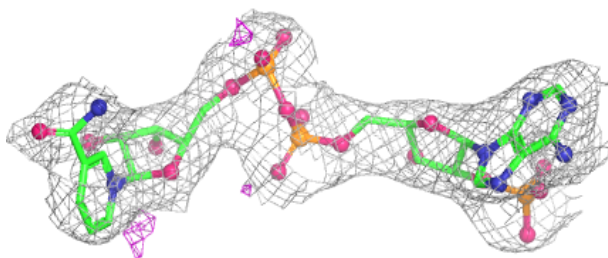
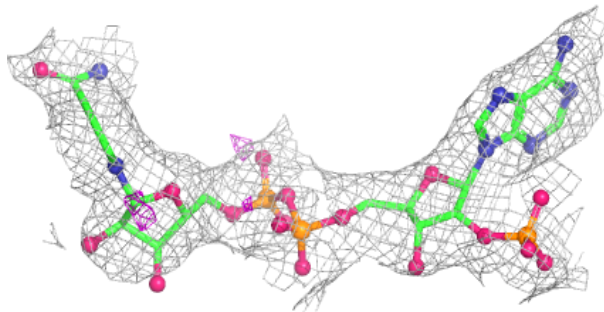


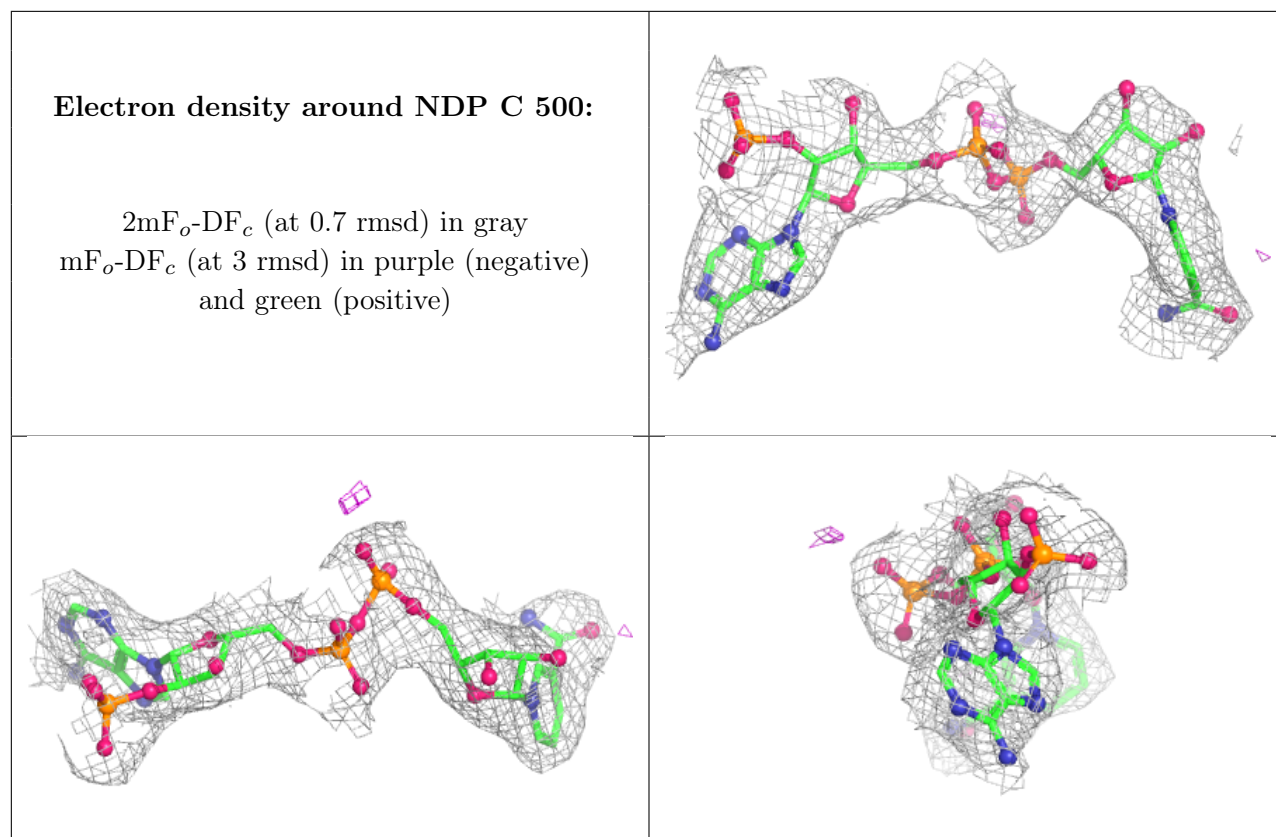
Electron density around NDP I 500:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.