



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:32 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

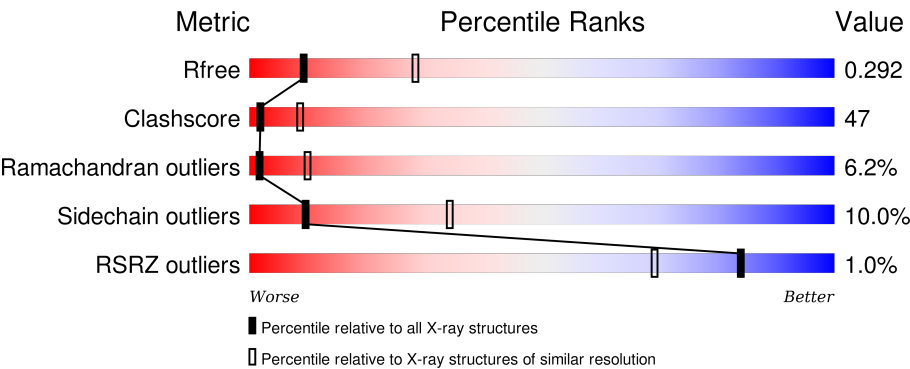
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>%</div><div><div></div><div>42%</div><div>44%</div><div>8%</div><div>5%</div></div></div>
1	B	384	<div><div></div><div>39%</div><div>43%</div><div>11%</div><div>7%</div></div>
1	D	384	<div><div>3%</div><div></div><div>29%</div><div>54%</div><div>13%</div><div></div></div>
1	E	384	<div><div>%</div><div></div><div>33%</div><div>51%</div><div>8%</div><div>7%</div></div>
1	G	384	<div><div></div><div>38%</div><div>49%</div><div>8%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
1	H	384	
2	C	174	
2	F	174	
2	I	174	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SUC	B	600	-	-	-	X
3	SUC	D	600	-	-	-	X
3	SUC	E	600	-	-	-	X
3	SUC	G	600	-	-	-	X
3	SUC	H	600	-	-	-	X
5	NAD	B	400	-	-	-	X

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:

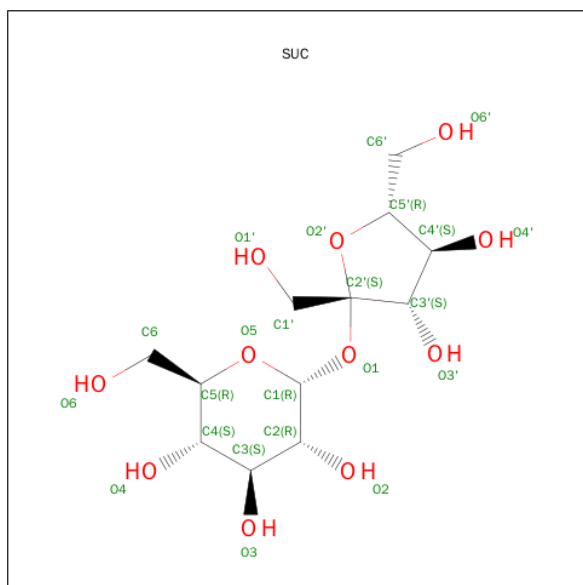
Chain	Residue	Modelled	Actual	Comment	Reference
C	291	ARG	-	CLONING ARTIFACT	UNP Q59765
C	292	HIS	-	CLONING ARTIFACT	UNP Q59765
C	293	MET	-	CLONING ARTIFACT	UNP Q59765
F	291	ARG	-	CLONING ARTIFACT	UNP Q59765
F	292	HIS	-	CLONING ARTIFACT	UNP Q59765
F	293	MET	-	CLONING ARTIFACT	UNP Q59765

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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 SUGAR (SUCROSE) (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 23 12 11	0	0
3	B	1	Total C O 23 12 11	0	0
3	D	1	Total C O 23 12 11	0	0
3	E	1	Total C O 23 12 11	0	0
3	G	1	Total C O 23 12 11	0	0
3	H	1	Total C O 23 12 11	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

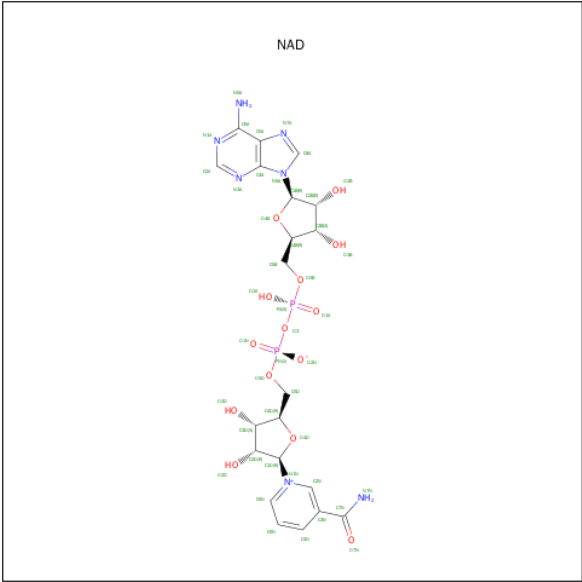
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

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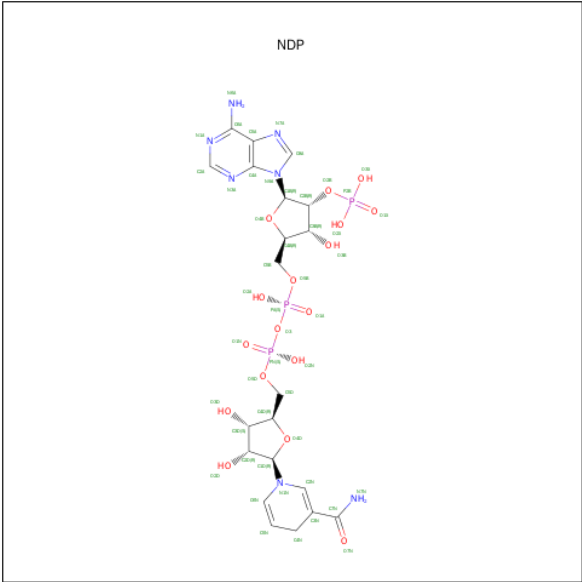
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 6 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

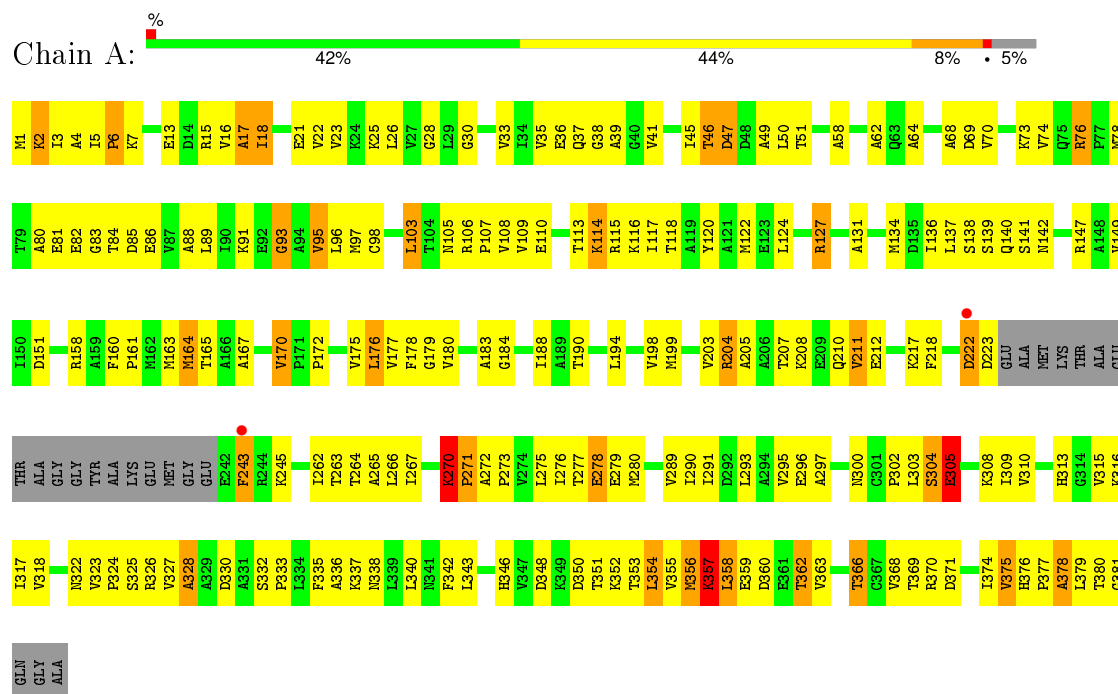


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
6	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
6	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

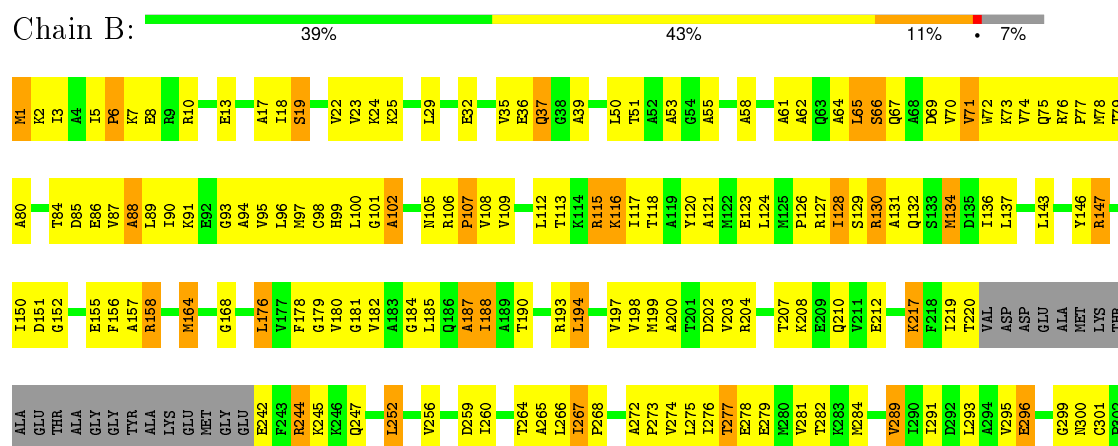
3 Residue-property plots

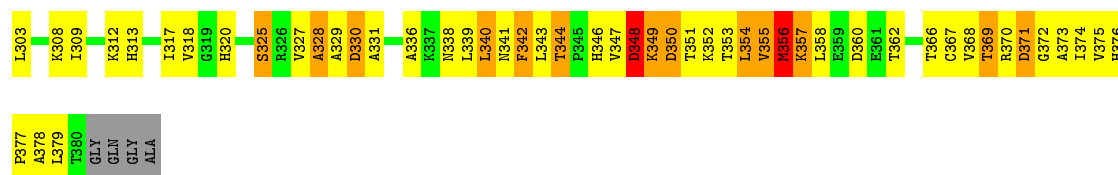
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

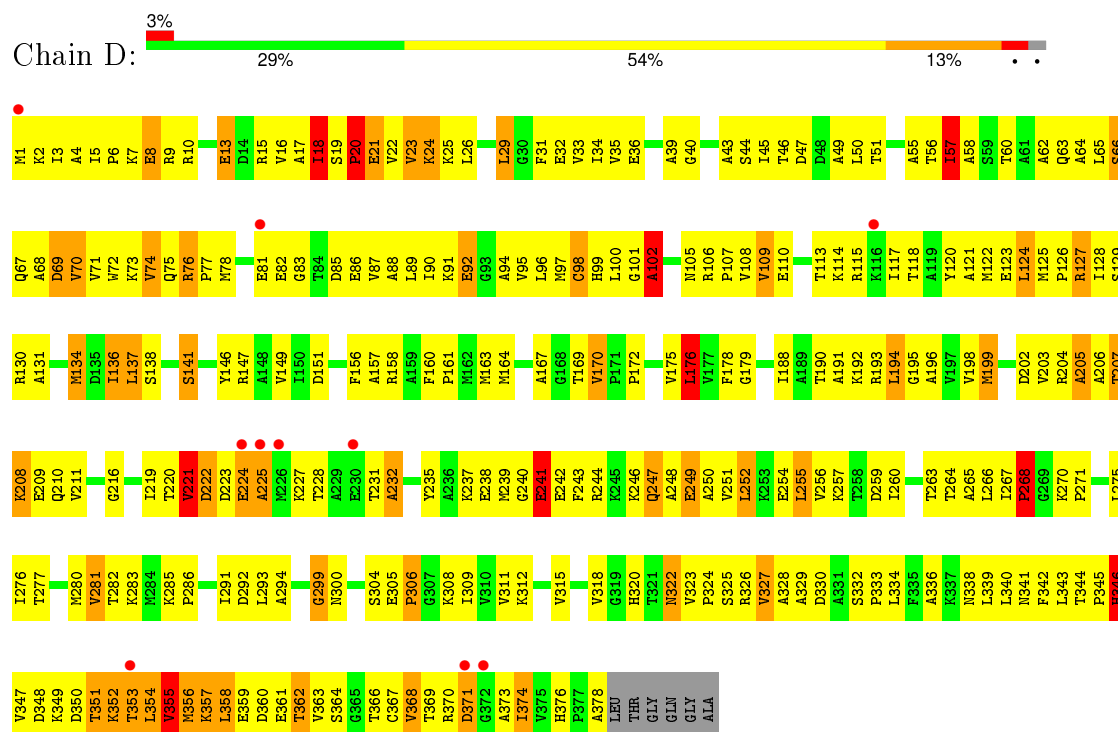


- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1

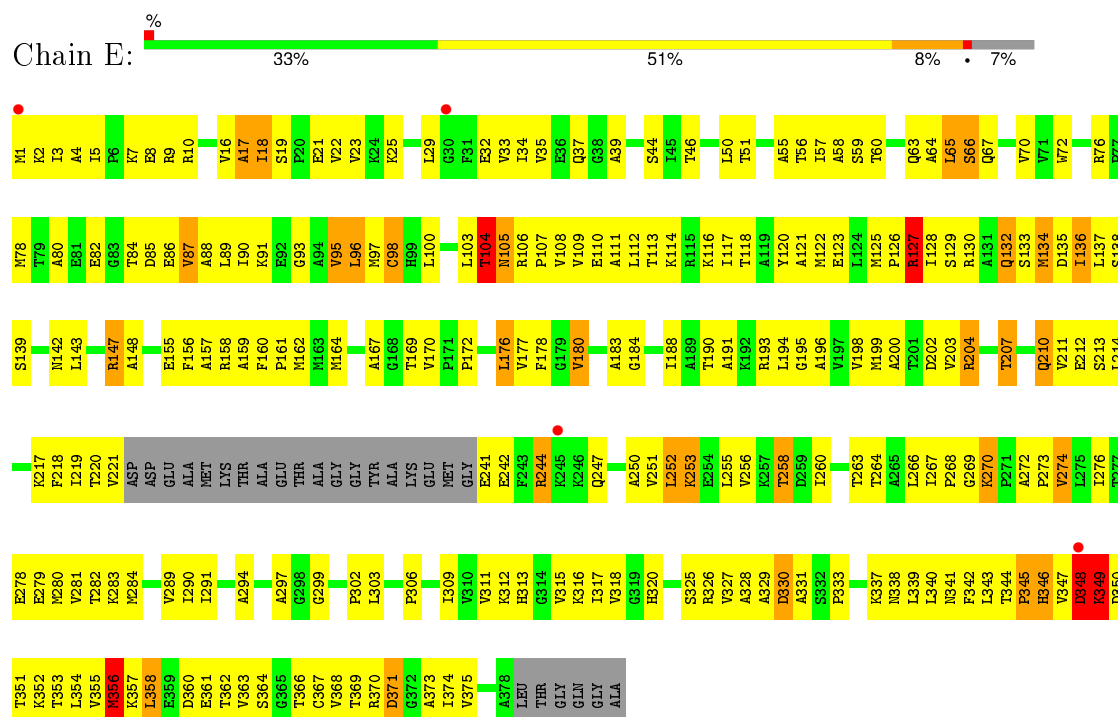




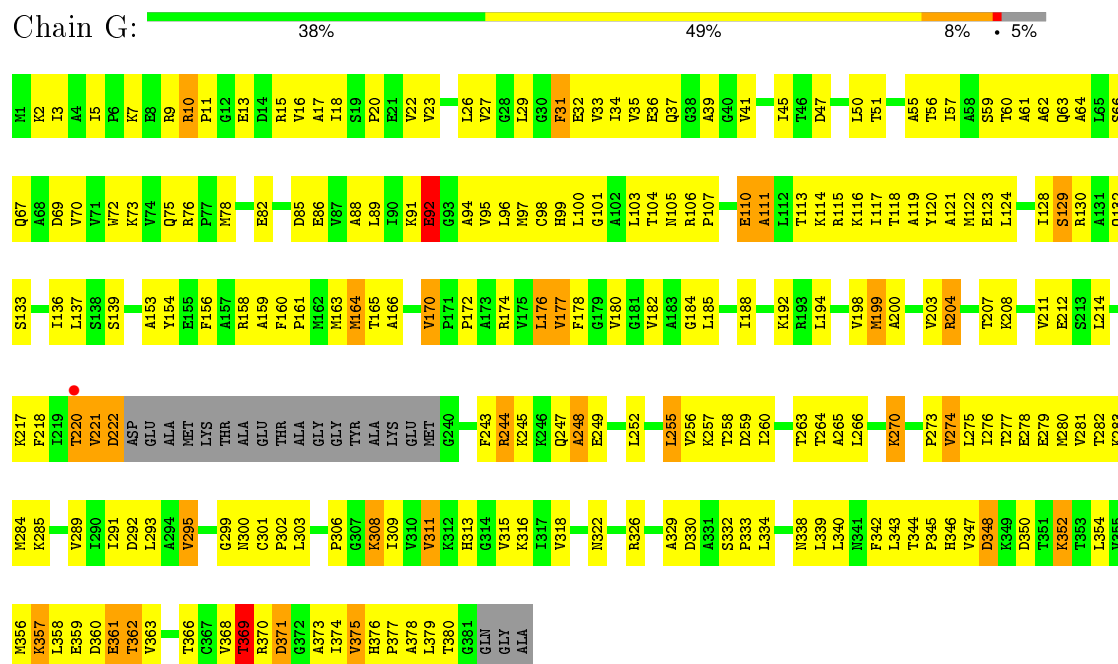
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



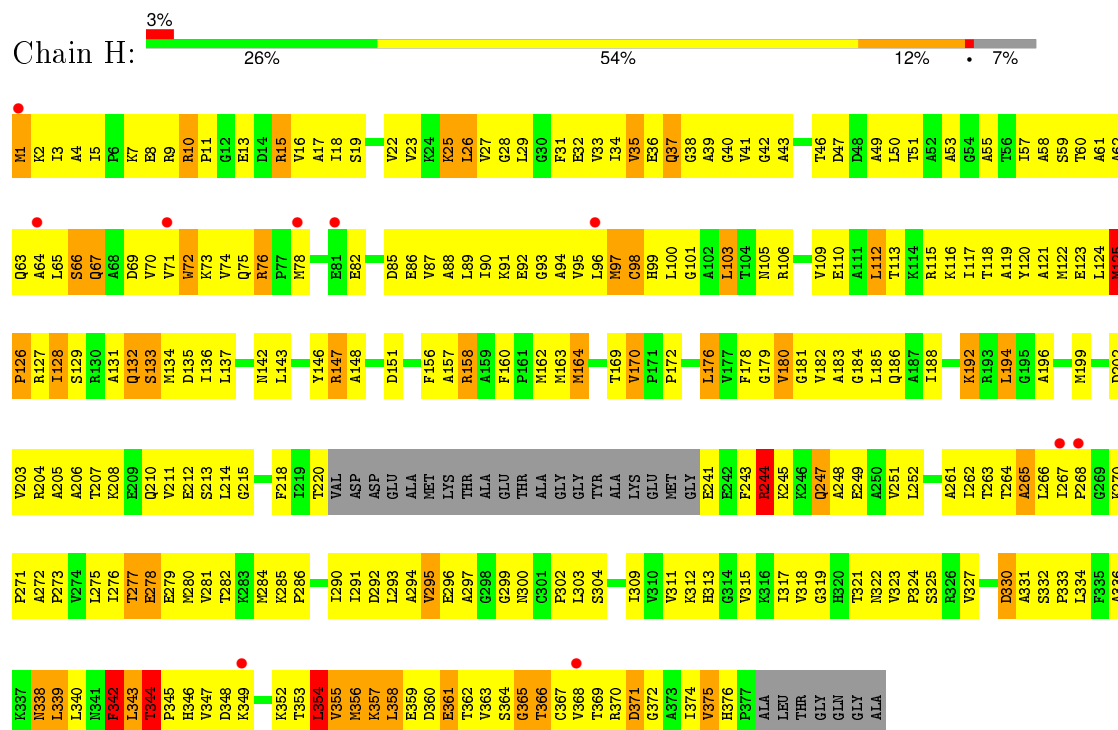
• Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



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

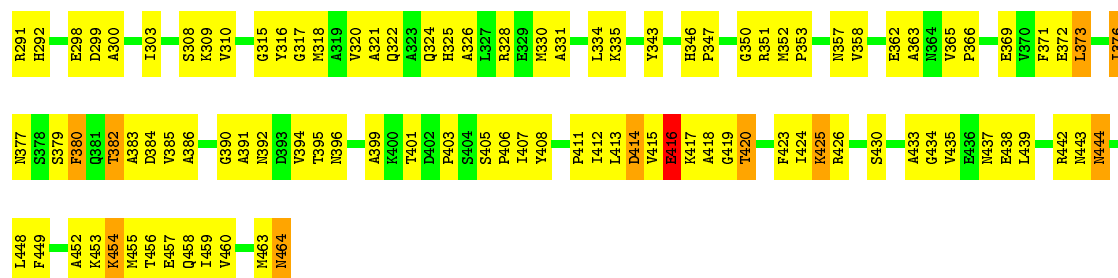


- Molecule 1: NAD(P) transhydrogenase subunit alpha part 1



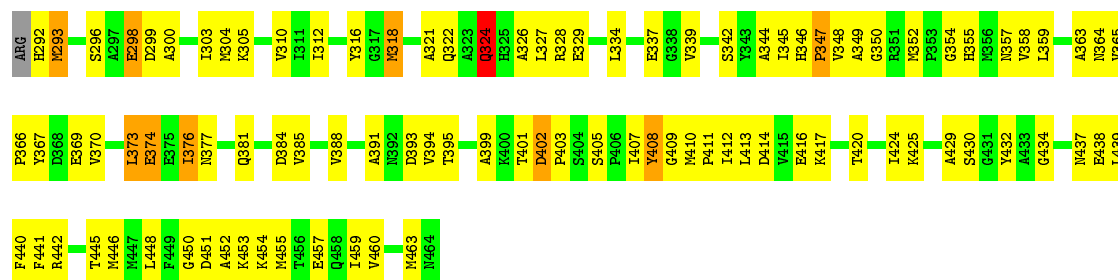
- Molecule 2: NAD(P) transhydrogenase subunit beta





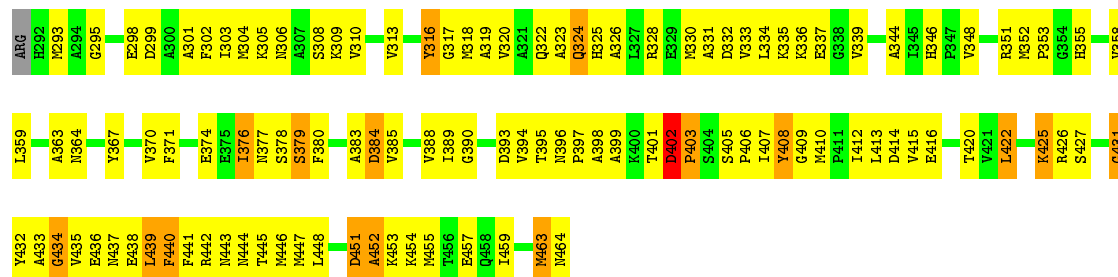
- Molecule 2: NAD(P) transhydrogenase subunit beta

Chain F: 44% 50% 5% ..



- Molecule 2: NAD(P) transhydrogenase subunit beta

Chain I: 34% 55% 9% ..



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 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.68-3.10) 95.9 (43.68-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.310 0.227 , 0.292	Depositor DCC
R_{free} test set	2977 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 64630 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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, SUC, NAD, NA

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

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

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

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

All (3) bond length outliers are listed below:

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

All (45) bond angle outliers are listed below:

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

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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	366	THR	CA

All (11) planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	22	0	0
3	B	23	0	22	1	0
3	D	23	0	22	0	0
3	E	23	0	22	0	0
3	G	23	0	22	0	0
3	H	23	0	22	1	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
5	A	44	0	26	2	0
5	B	44	0	25	9	0
5	D	44	0	24	3	0
5	G	44	0	24	6	0
5	H	44	0	26	8	0
6	C	48	0	26	4	0
6	F	48	0	26	10	0
6	I	48	0	26	3	0
All	All	20480	0	21071	1966	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:120:TYR:CD2	1:H:366:THR:HG22	1.64	1.31
1:H:120:TYR:HD2	1:H:366:THR:CG2	1.47	1.27
2:I:401:THR:O	2:I:403:PRO:HD3	1.32	1.25
1:B:70:VAL:HG23	1:B:95:VAL:HB	1.21	1.17
1:H:120:TYR:CD2	1:H:366:THR:CG2	2.26	1.15
1:D:62:ALA:HA	1:D:89:LEU:HD21	1.16	1.11
1:H:18:ILE:HD11	1:H:23:VAL:HG22	1.23	1.10
1:H:120:TYR:HD2	1:H:366:THR:HG22	0.94	1.09
1:B:264:THR:HG22	1:B:293:LEU:HD12	1.33	1.08
1:B:29:LEU:HD23	1:B:347:VAL:HG11	1.35	1.08
1:B:86:GLU:HA	1:B:89:LEU:HD12	1.37	1.07
1:A:270:LYS:HB2	1:A:271:PRO:HD3	1.37	1.06
1:H:47:ASP:HB3	1:H:57:ILE:HD13	1.34	1.05
1:H:72:TRP:HB3	1:H:97:MET:HB2	1.34	1.04
1:H:47:ASP:HB3	1:H:57:ILE:CD1	1.87	1.04
1:H:370:ARG:CG	1:H:375:VAL:HG21	1.88	1.04

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:VAL:HG21	1:H:50:LEU:HD23	1.52	0.92
2:F:401:THR:O	2:F:403:PRO:HD3	1.69	0.92
1:H:78:MET:HB2	1:H:86:GLU:HB2	1.49	0.91
1:D:247:GLN:HE22	5:D:400:NAD:H61A	1.19	0.91
2:I:399:ALA:HA	2:I:408:TYR:HA	1.53	0.91
1:H:72:TRP:CZ3	1:H:339:LEU:HB3	2.06	0.91
1:D:163:MET:HE1	1:E:142:ASN:HD21	1.34	0.91
1:A: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: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
2:C:464:ASN:HD22	2:C:464:ASN:C	1.77	0.88
1:H:122:MET:H	1:H:122:MET:HE2	1.38	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
1:H:119:ALA:O	1:H:367:CYS:HA	1.74	0.86
2:F:324:GLN:NE2	2:F:359:LEU:HD22	1.90	0.86
1:D:88:ALA:HA	1:D:115:ARG:HD2	1.57	0.86
1:H:129:SER:HA	1:H:132:GLN:CG	2.05	0.86
1:D:342:PHE:O	1:D:345:PRO:HD2	1.75	0.86
1:D:270:LYS:HE2	1:D:270:LYS:HA	1.57	0.86
1:E:278:GLU:O	1:E:281:VAL:HG12	1.75	0.86
1:H:120:TYR:HA	1:H:366:THR:HG23	1.56	0.86
2:I:399:ALA:HB2	2:I:407:ILE:HG13	1.57	0.86
1:A:289:VAL:HG22	1:A:316:LYS:HB2	1.56	0.86
1:G:72:TRP:HE1	1:G:97:MET:HE1	1.36	0.86
1:H:18:ILE:HD11	1:H:23:VAL:CG2	2.05	0.85
1:H:10:ARG:HH21	1:H:78:MET:HA	1.38	0.85
1:D:329:ALA:HB3	1:E:158:ARG:HG3	1.59	0.85
1:H:243:PHE:O	1:H:247:GLN:HB3	1.75	0.85
1:D:21:GLU:CD	2:I:308:SER:HB2	1.97	0.85
1:H:10:ARG:NH2	1:H:78:MET:HA	1.92	0.85
2:C:392:ASN:O	2:C:395:THR:HG22	1.76	0.85
1:A:105:ASN:O	1:A:108:VAL:HG12	1.76	0.84
1:D:70:VAL:HG12	1:D:95:VAL:HB	1.58	0.84
1:A:265:ALA:HB3	1:A:300:ASN:ND2	1.93	0.84
1:D:175:VAL:HG12	1:D:176:LEU:H	1.43	0.83
1:H:367:CYS:SG	1:H:370:ARG:HD3	2.18	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:LYS:O	1:D:249:GLU:HB3	1.78	0.83
1:A:277:THR:H	1:A:280:MET:CE	1.91	0.83
1:H:136:ILE:HG13	1:H:137:LEU:N	1.93	0.83
1:G:376:HIS:O	1:G:380:THR:HG22	1.78	0.83
1:D:270:LYS:HB3	1:D:271:PRO:HD2	1.60	0.83
1:D:68:ALA:O	1:D:91:LYS:CD	2.27	0.83
1:E:253:LYS:O	1:E:253:LYS:HE3	1.78	0.83
1:E:349:LYS:HG3	1:E:349:LYS:O	1.77	0.82
1:E:90:ILE:HD13	1:E:117:ILE:HD13	1.61	0.82
2:F:432:TYR:CE2	6:F:500:NDP:H6N	2.14	0.82
1:G:158:ARG:HB2	1:H:330:ASP:OD2	1.80	0.82
1:H:93:GLY:HA2	1:H:116:LYS:HB2	1.61	0.82
1:B:340:LEU:O	1:B:344:THR:HG23	1.79	0.82
1:G:256:VAL:HG12	1:G:283:LYS:O	1.79	0.82
1:E:87:VAL:HG23	1:E:112:LEU:HG	1.62	0.81
1:E:358:LEU:HD12	1:E:358:LEU:H	1.43	0.81
1:A:291:ILE:HD13	1:A:318:VAL:HB	1.61	0.81
1:H:61:ALA:HB1	1:H:89:LEU:HD13	1.61	0.81
1:D:239:MET:HB2	1:D:244:ARG:HE	1.44	0.81
1:G:115:ARG:NH2	1:G:115:ARG:HB3	1.96	0.81
1:D:160:PHE:O	1:D:172:PRO:HA	1.81	0.81
2:I:403:PRO:HA	2:I:408:TYR:CG	2.16	0.81
1:D:354:LEU:HD21	1:D:356:MET:SD	2.20	0.81
1:H:136:ILE:HA	1:H:338:ASN:OD1	1.80	0.81
1:H:67:GLN:H	1:H:67:GLN:NE2	1.78	0.81
1:A:58:ALA:HB3	1:A:64:ALA:HB2	1.62	0.81
1:D:294:ALA:HB3	1:D:300:ASN:OD1	1.81	0.80
1:D:5:ILE:HG23	1:D:72:TRP:O	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:G:163:MET:HB2	1:G:170:VAL:CG1	2.11	0.80
1:B:8:GLU:CD	1:B:74:VAL:HG22	2.01	0.80
1:H:106:ARG:O	1:H:109:VAL:HG12	1.82	0.80
1:D:92:GLU:HB2	1:D:115:ARG:O	1.81	0.79
2:I:451:ASP:OD1	2:I:453:LYS:HB3	1.82	0.79
1:G:221:VAL:HG11	1:G:243:PHE:CZ	2.17	0.79
1:H:67:GLN:HA	1:H:91:LYS:HE3	1.62	0.79
2:C:454:LYS:HE2	2:C:454:LYS:HA	1.65	0.79
1:E:255:LEU:HA	1:E:258:THR:OG1	1.82	0.79
2:I:305:LYS:HE2	2:I:337:GLU:OE1	1.82	0.79
1:D:90:ILE:HD13	1:D:117:ILE:HD13	1.63	0.79

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:264:THR:HG22	1:G:293:LEU:HD12	1.68	0.75
1:D:368:VAL:HA	1:D:376:HIS:HB2	1.69	0.75
2:I:437:ASN:HB3	2:I:440:PHE:HE1	1.49	0.75
1:D:291:ILE:N	1:D:291:ILE:HD12	2.02	0.75
1:A:106:ARG:N	1:A:107:PRO:HD2	2.01	0.75
2:F:354:GLY:O	2:F:358:VAL:HG23	1.86	0.75
1:D:203:VAL:HG12	1:D:243:PHE:HE2	1.51	0.75
1:E:60:THR:CG2	1:E:63:GLN:HG3	2.16	0.75
1:D:369:THR:HA	1:D:373:ALA:O	1.87	0.75
1:G:120:TYR:HB3	1:G:366:THR:CG2	2.15	0.75
1:D:3:ILE:O	1:D:33:VAL:HA	1.87	0.74
1:H:142:ASN:HD22	2:I:353:PRO:HD2	1.50	0.74
1:B:369:THR:HB	1:B:374:ILE:HA	1.68	0.74
1:A:165:THR:HG22	2:C:353:PRO:HB3	1.70	0.74
1:D:276:ILE:HA	1:D:280:MET:HE3	1.69	0.74
1:A:368:VAL:HA	1:A:376:HIS:HB2	1.69	0.74
2:F:348:VAL:HG21	2:F:410:MET:HE1	1.69	0.74
2:I:425:LYS:HD3	2:I:427:SER:O	1.88	0.74
2:I:295:GLY:HA3	2:I:446:MET:HE2	1.70	0.73
2:F:328:ARG:HD3	2:F:363:ALA:O	1.88	0.73
1:H:74:VAL:HG23	1:H:75:GLN:N	2.03	0.73
2:F:432:TYR:CZ	6:F:500:NDP:H6N	2.23	0.73
1:H:184:GLY:O	1:H:188:ILE:HG13	1.88	0.73
1:D:10:ARG:HH21	1:D:10:ARG:HG3	1.52	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:217:LYS:N	1:E:217:LYS:HD2	2.04	0.73
1:E:66:SER:O	1:E:91:LYS:HB2	1.89	0.73
1:D:308:LYS:HG2	1:D:309:ILE:H	1.51	0.73
1:B:368:VAL:HA	1:B:376:HIS:HB2	1.70	0.72
1:B:113:THR:HG23	1:B:373:ALA:HA	1.70	0.72
1:H:116:LYS:HA	1:H:372:GLY:N	2.04	0.72
1:G:2:LYS:HA	1:G:32:GLU:HB2	1.70	0.72
1:G:62:ALA:HB2	1:G:89:LEU:HD23	1.71	0.72
1:D:163:MET:HB2	1:D:170:VAL:HG13	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:H:367:CYS:SG	1:H:370:ARG:CD	2.77	0.72
1:E:244:ARG:CB	1:E:244:ARG:HH21	2.02	0.72
1:H:61:ALA:O	1:H:89:LEU:HB3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:ASN:O	1:E:345:PRO:HD3	1.90	0.72
1:H:93:GLY:CA	1:H:116:LYS:HB2	2.20	0.72
2:C:454:LYS:O	2:C:458:GLN:HG3	1.90	0.72
1:H:186:GLN:HA	2:I:352:MET:CE	2.16	0.72
1:B:118:THR:HA	1:B:369:THR:O	1.89	0.72
1:G:347:VAL:HG12	1:G:348:ASP:O	1.89	0.72
1:D:264:THR:HG22	1:D:293:LEU:HD12	1.72	0.72
1:D:23:VAL:HG11	1:D:55:ALA:HB2	1.71	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:A:276:ILE:HA	1:A:280:MET:CE	2.21	0.71
1:G:166:ALA:HB1	1:H:133:SER:HA	1.71	0.71
1:H:180:VAL:HG11	1:H:207:THR:HG23	1.71	0.71
1:E:312:LYS:HE3	1:E:313:HIS:NE2	2.05	0.71
1:A:278:GLU:HB2	1:A:303:LEU:HD11	1.72	0.71
1:B:147:ARG:HD2	1:B:151:ASP:OD2	1.91	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
1:D:293:LEU:CD2	1:D:323:VAL:HG21	2.21	0.71
1:D:285:LYS:HD3	1:D:286:PRO:N	2.04	0.71
1:H:368:VAL:O	1:H:375:VAL:N	2.21	0.71
2:C:322:GLN:NE2	2:C:324:GLN:HE22	1.89	0.71
1:E:244:ARG:HB3	1:E:244:ARG:HH21	1.56	0.71
1:H:93:GLY:HA2	1:H:116:LYS:O	1.90	0.70
1:H:202:ASP:HA	5:H:400:NAD:H8A	1.71	0.70
1:G:275:LEU:HB2	1:G:300:ASN:HB3	1.72	0.70
1:G:106:ARG:N	1:G:107:PRO:HD2	2.05	0.70
1:H:120:TYR:CD2	1:H:366:THR:HG21	2.23	0.70
1:A:76:ARG:NH2	1:A:76:ARG:HG2	1.97	0.70
1:H:120:TYR:CA	1:H:366:THR:HG23	2.21	0.70
1:D:207:THR:HA	1:D:210:GLN:HE21	1.56	0.70
1:B:346:HIS:O	1:B:355:VAL:HG12	1.91	0.70
1:D:120:TYR:HD1	1:D:366:THR:O	1.75	0.70
1:E:25:LYS:O	1:E:29:LEU:HD13	1.92	0.70
1:D:357:LYS:O	1:D:359:GLU:HG3	1.90	0.70
1:E:125:MET:HE3	1:E:342:PHE:HD2	1.57	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:B:94:ALA:O	1:B:117:ILE:HG23	1.91	0.70
1:D:265:ALA:O	1:D:266:LEU:HD23	1.90	0.70
1:B:3:ILE:HG13	1:B:70:VAL:HG13	1.74	0.70

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:GLN:HE21	1:H:248:ALA:N	1.93	0.67
2:F:381:GLN:HG2	2:F:417:LYS:HE2	1.76	0.66
1:G:78:MET:H	1:G:86:GLU:HB2	1.59	0.66
1:H:69:ASP:O	1:H:95:VAL:HG23	1.95	0.66
1:B:108:VAL:O	1:B:112:LEU:HD13	1.94	0.66
1:G:263:THR:OG1	1:G:292:ASP:HA	1.95	0.66
1:H:110:GLU:HA	1:H:374:ILE:HD11	1.77	0.66
1:H:218:PHE:HD2	1:H:220:THR:HG23	1.59	0.66
2:C:310:VAL:HG22	2:C:385:VAL:HB	1.77	0.66
1:B:349:LYS:HG3	1:B:350:ASP:N	2.07	0.66
1:H:284:MET:SD	1:H:290:ILE:HD11	2.36	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: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
2:C:309:LYS:NZ	2:C:382:THR:HB	2.11	0.66
1:H:264:THR:HG22	1:H:293:LEU:HD12	1.78	0.66
1:A:277:THR:H	1:A:280:MET:HE2	1.60	0.66
1:G:359:GLU:CD	1:G:359:GLU:H	1.99	0.66
1:H:346:HIS:HB3	1:H:356:MET:HB3	1.78	0.66
1:D:20:PRO:HD3	1:D:45:ILE:HG21	1.78	0.66
2:F:446:MET:HE3	2:F:448:LEU:HD21	1.78	0.66
1:E:284:MET:HE1	1:E:315:VAL:HG11	1.77	0.66
1:A:93:GLY:HA2	1:A:116:LYS:O	1.95	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:H:178:PHE:CE1	1:H:276:ILE:HD11	2.30	0.65
1:G:362:THR:HG22	1:G:363:VAL:N	2.11	0.65
1:E:60:THR:HG22	1:E:63:GLN:HG3	1.76	0.65
1:D:96:LEU:HD23	1:D:96:LEU:O	1.96	0.65
1:D:87:VAL:O	1:D:115:ARG:CD	2.44	0.65
1:B:267:ILE:CD1	5:B:400:NAD:N1A	2.59	0.65
1:D:354:LEU:C	1:D:355:VAL:HG22	2.16	0.65
1:G:113:THR:HG23	1:G:373:ALA:HA	1.78	0.65
2:C:433:ALA:O	2:C:435:VAL:HG23	1.96	0.65
1:B:136:ILE:HA	1:B:338:ASN:OD1	1.97	0.65
1:H:355:VAL:O	1:H:355:VAL:HG13	1.95	0.65
2:I:401:THR:C	2:I:403:PRO:HD3	2.15	0.65
1:D:277:THR:H	1:D:280:MET:HE3	1.62	0.65
1:H:136:ILE:HG13	1:H:137:LEU:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:LEU:H	1:D:50:LEU:HD12	1.61	0.65
1:H:5:ILE:HB	1:H:35:VAL:HG12	1.79	0.65
1:D:322:ASN:ND2	1:D:325:SER:HB2	2.11	0.65
1:H:7:LYS:HB2	1:H:39:ALA:HA	1.79	0.65
1:G:120:TYR:OH	1:G:356:MET:HG3	1.97	0.65
1:G:362:THR:HG22	1:G:363:VAL:H	1.61	0.65
1:G:89:LEU:H	1:G:89:LEU:HD12	1.60	0.65
1:A:167:ALA:HB2	1:B:338:ASN:HD21	1.62	0.65
1:B:136:ILE:HG13	1:B:137:LEU:HD12	1.77	0.65
1:D:97:MET:HB2	1:D:122:MET:CE	2.27	0.65
1:G:5:ILE:HB	1:G:35:VAL:HG12	1.79	0.65
1:A:136:ILE:HG13	1:A:137:LEU:N	2.12	0.65
2:I:432:TYR:C	2:I:434:GLY:H	1.98	0.64
2:F:304:MET:HG2	2:F:385:VAL:HG11	1.79	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:F:454:LYS:HA	2:F:457:GLU:OE1	1.96	0.64
2:C:420:THR:HB	1:H:162:MET:CE	2.28	0.64
1:H:281:VAL:HG11	1:H:303:LEU:HD12	1.79	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:5:ILE:HG13	1:H:72:TRP:CD1	2.33	0.64
1:D:88:ALA:HA	1:D:115:ARG:CD	2.27	0.64
1:H:247:GLN:NE2	1:H:248:ALA:N	2.45	0.64
1:H:208:LYS:NZ	1:H:220:THR:HG21	2.12	0.64
1:H:241:GLU:O	1:H:245:LYS:HG2	1.97	0.64
1:E:128:ILE:HD11	1:E:130:ARG:HH21	1.63	0.64
1:B:143:LEU:HD12	1:B:331:ALA:HB2	1.78	0.64
1:B:29:LEU:CD2	1:B:347:VAL:HG11	2.21	0.64
1:B:10:ARG:HH11	1:B:10:ARG:HG3	1.62	0.64
1:H:162:MET:HB2	1:H:172:PRO:HD3	1.80	0.64
1:G:67:GLN:HA	1:G:91:LYS:HD3	1.80	0.64
1:G:66:SER:O	1:G:91:LYS:HB3	1.98	0.64
1:A:304:SER:O	1:A:305:GLU:C	2.36	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:A:207:THR:HG22	1:A:218:PHE:HE1	1.63	0.64
1:B:180:VAL:HG23	1:B:202:ASP:HB2	1.79	0.64
1:G:273:PRO:HG3	5:G:400:NAD:H2A	1.80	0.63
2:F:366:PRO:HB2	2:F:369:GLU:HG3	1.80	0.63
1:B:264:THR:CG2	1:B:293:LEU:HD12	2.20	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:HIS:CD2	1:D:356:MET:HA	2.34	0.63
1:D:246:LYS:O	1:D:249:GLU:CB	2.46	0.63
1:B:126:PRO:HG2	1:B:362:THR:HA	1.80	0.63
1:A:6:PRO:HA	1:A:36:GLU:HG2	1.81	0.63
1:B:376:HIS:HB3	1:B:379:LEU:HD13	1.80	0.63
1:E:136:ILE:CD1	1:E:137:LEU:HD12	2.28	0.63
1:D:106:ARG:O	1:D:109:VAL:HG22	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:375:VAL:O	1:A:375:VAL:HG22	1.98	0.63
1:G:120:TYR:CE2	1:G:363:VAL:HG13	2.33	0.63
1:A:180:VAL:HG11	1:A:207:THR:HG23	1.80	0.63
1:B:86:GLU:O	1:B:89:LEU:HB2	1.98	0.63
1:G:282:THR:HG22	1:G:313:HIS:HD2	1.64	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:H:122:MET:CE	1:H:122:MET:H	2.12	0.63
1:E:362:THR:CG2	1:E:363:VAL:N	2.60	0.63
2:I:410:MET:O	2:I:410:MET:HG3	1.99	0.63
1:A:276:ILE:HA	1:A:280:MET:HE3	1.81	0.63
1:D:3:ILE:HB	1:D:70:VAL:HG23	1.81	0.63
2:C:424:ILE:O	2:C:424:ILE:HG22	1.99	0.63
1:E:89:LEU:H	1:E:89:LEU:HD12	1.64	0.63
1:A:376:HIS:HD2	1:A:378:ALA:CB	2.12	0.63
1:H:120:TYR:HB3	1:H:366:THR:HG21	1.80	0.62
1:B:5:ILE:N	1:B:5:ILE:HD12	2.14	0.62
1:E:34:ILE:CD1	1:E:56:THR:HB	2.28	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:G:5:ILE:N	1:G:5:ILE:HD12	2.14	0.62
1:D:277:THR:H	1:D:280:MET:CE	2.12	0.62
1:D:2:LYS:HD2	1:D:32:GLU:HB3	1.81	0.62
1:E:86:GLU:C	1:E:88:ALA:H	2.03	0.62
1:B:147:ARG:CD	1:B:151:ASP:OD2	2.47	0.62
1:H:272:ALA:HB1	1:H:273:PRO:HD2	1.80	0.62
2:F:344:ALA:HB2	2:F:376:ILE:HD13	1.82	0.62
1:H:362:THR:CG2	1:H:363:VAL:H	2.07	0.62
1:D:163:MET:HE1	1:E:142:ASN:ND2	2.11	0.62
2:I:377:ASN:O	2:I:379:SER:N	2.31	0.62
1:H:276:ILE:O	1:H:302:PRO:HD2	1.99	0.62
1:D:178:PHE:CE2	1:D:276:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:O	1:B:256:VAL:HG23	2.00	0.61
1:A:342:PHE:CE1	1:A:362:THR:HG23	2.34	0.61
1: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
1:D:194:LEU:HD21	1:E:194:LEU:HD13	1.82	0.61
1:E:348:ASP:CG	1:E:351:THR:HB	2.20	0.61
2:C:395:THR:HG23	2:C:437:ASN:HD21	1.64	0.61
1:H:60:THR:HG23	1:H:63:GLN:H	1.63	0.61
2:I:330:MET:HG3	2:I:463:MET:HE3	1.82	0.61
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
2:C:464:ASN:ND2	2:C:464:ASN:C	2.48	0.61
1:G:257:LYS:HA	1:G:285:LYS:HE3	1.82	0.61
1:G:243:PHE:O	1:G:247:GLN:HB3	2.00	0.61
1:A:163:MET:HB2	1:A:170:VAL:CG1	2.29	0.61
1:B:274:VAL:CG1	1:B:277:THR:HG23	2.31	0.61
1:A:322:ASN:ND2	1:A:325:SER:HB2	2.14	0.61
2:C:316:TYR:O	2:C:320:VAL:HG23	2.00	0.61
2:I:437:ASN:CB	2:I:440:PHE:HE1	2.13	0.61
1:G:376:HIS:HD2	1:G:378:ALA:CB	2.13	0.61
1:H:34:ILE:HG23	1:H:58:ALA:HB2	1.82	0.61
1:B:96:LEU:HD23	1:B:112:LEU:HD21	1.82	0.61
1:G:326:ARG:HH21	1:G:326:ARG:HG2	1.66	0.61
1:E:16:VAL:HG22	1:E:18:ILE:HG22	1.82	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: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
1:D:136:ILE:HD13	1:D:137:LEU:N	2.16	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:G:36:GLU:OE1	1:G:61:ALA:HB2	2.01	0.61
1:D:5:ILE:HG12	1:D:18:ILE:HB	1.82	0.61
1:B:1:MET:CE	1:B:353:THR:HA	2.30	0.61
2:I:308:SER:HB3	2:I:384:ASP:OD2	2.00	0.61
1:H:2:LYS:HD3	1:H:32:GLU:HB2	1.82	0.61
1:G:139:SER:HB2	1:G:334:LEU:HD23	1.82	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:374:ILE:HD12	1:G:374:ILE:H	1.66	0.61
1:H:64:ALA:C	1:H:65:LEU:HD12	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:310:VAL:HG22	2:F:385:VAL:HB	1.83	0.61
1:H:120:TYR:CB	1:H:366:THR:CG2	2.79	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:H:208:LYS:HZ2	1:H:220:THR:HG21	1.66	0.61
1:D:285:LYS:C	1:D:285:LYS:HD3	2.22	0.61
2:I:403:PRO:HA	2:I:408:TYR:CD2	2.35	0.60
1:E:342:PHE:CD1	1:E:342:PHE:O	2.54	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
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:B:312:LYS:HG2	1:B:313:HIS:CD2	2.36	0.60
1:D:76:ARG:HG2	1:D:100:LEU:HA	1.83	0.60
1:D:131:ALA:HB1	1:D:134:MET:HG3	1.83	0.60
1:H:47:ASP:HB2	1:H:57:ILE:CD1	2.32	0.60
1:H:112:LEU:HD12	1:H:112:LEU:N	2.15	0.60
1:D:97:MET:HB2	1:D:122:MET:HE1	1.84	0.60
1:G:9:ARG:NH2	1:G:36:GLU:OE2	2.34	0.60
1:E:125:MET:HE3	1:E:134:MET:SD	2.42	0.60
1:H:70:VAL:HA	1:H:95:VAL:HB	1.83	0.60
1:G:221:VAL:HG12	1:G:222:ASP:N	2.16	0.60
1:E:360:ASP:CG	1:E:362:THR:HG22	2.21	0.60
1:H:163:MET:HB2	1:H:170:VAL:HG23	1.83	0.60
1:D:50:LEU:O	1:D:55:ALA:HB3	2.02	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:E:284:MET:CE	1:E:290:ILE:HD11	2.32	0.60
1:A:141:SER:O	1:A:183:ALA:HB2	2.01	0.60
2:C:373:LEU:HD23	2:C:373:LEU:C	2.22	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:D:91:LYS:O	1:D:92:GLU:C	2.40	0.60
1:D:265:ALA:HB3	1:D:300:ASN:HD21	1.67	0.60
1:B:118:THR:HG23	1:B:370:ARG:HB3	1.83	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:HG22	1:G:104:THR:O	2.02	0.60
1:H:87:VAL:HG21	1:H:112:LEU:HA	1.83	0.59
1:D:342:PHE:CE1	1:D:362:THR:HG23	2.37	0.59
1:G:10:ARG:HG2	1:G:75:GLN:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ARG:HH21	1:G:115:ARG:CB	2.13	0.59
2:C:321:ALA:CB	2:C:452:ALA:HB3	2.31	0.59
1:E:138:SER:OG	1:E:139:SER:N	2.35	0.59
1:G:311:VAL:HG13	1:G:316:LYS:HG2	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:277:THR:H	1:A:280:MET:HE3	1.65	0.59
1:H:28:GLY:C	1:H:29:LEU:HD12	2.22	0.59
1:B:146:TYR:CE2	1:B:150:ILE:HG13	2.37	0.59
1:H:142:ASN:ND2	2:I:353:PRO:HB2	2.17	0.59
1:G:2:LYS:O	1:G:69:ASP:HB2	2.03	0.59
1:B:99:HIS:CD2	1:B:101:GLY:H	2.19	0.59
1:G:374:ILE:HD12	1:G:374:ILE:N	2.17	0.59
1:H:147:ARG:NH1	1:H:151:ASP:OD1	2.35	0.59
1:A:13:GLU:OE2	1:A:15:ARG:HB2	2.02	0.59
1:H:131:ALA:HA	1:H:134:MET:CE	2.32	0.59
1:G:128:ILE:HD12	1:G:129:SER:H	1.67	0.59
1:D:280:MET:C	1:D:282:THR:H	2.05	0.59
1:A:106:ARG:HH12	1:A:379:LEU:HG	1.65	0.59
1:H:162:MET:HE2	1:H:164:MET:SD	2.42	0.59
1:D:221:VAL:HG11	1:D:250:ALA:HB3	1.82	0.59
1:D:13:GLU:OE1	1:D:322:ASN:ND2	2.36	0.59
1:H:4:ALA:O	1:H:71:VAL:HG23	2.03	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:E:219:ILE:HG22	1:E:219:ILE:O	2.02	0.59
1:G:78:MET:HA	1:G:82:GLU:OE1	2.02	0.59
1:G:37:GLN:NE2	1:G:59:SER:HA	2.17	0.59
1:G:34:ILE:HD13	1:G:56:THR:HB	1.83	0.59
1:H:72:TRP:HA	1:H:97:MET:O	2.02	0.59
1:D:5:ILE:N	1:D:5:ILE:HD12	2.18	0.59
1:H:347:VAL:C	1:H:355:VAL:HG12	2.23	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:B:7:LYS:HG3	1:B:39:ALA:HA	1.85	0.59
1:H:7:LYS:HB2	1:H:39:ALA:CB	2.33	0.59
1:G:5:ILE:HG12	1:G:18:ILE:HB	1.85	0.59
1:A:58:ALA:CB	1:A:64:ALA:HB2	2.33	0.59
1:E:60:THR:HG23	1:E:63:GLN:H	1.67	0.59
2:F:437:ASN:C	2:F:439:LEU:H	2.06	0.59
2:I:346:HIS:CD2	2:I:394:VAL:HB	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLN:HA	1:H:91:LYS:CE	2.32	0.58
1:A:131:ALA:HA	1:A:134:MET:HE2	1.83	0.58
1:D:360:ASP:OD2	1:D:362:THR:HB	2.04	0.58
1:D:73:LYS:O	1:D:98:CYS:CB	2.45	0.58
1:G:120:TYR:HE2	1:G:363:VAL:HG13	1.67	0.58
1:E:76:ARG:HD2	1:E:108:VAL:HG21	1.85	0.58
2:C:346:HIS:HD2	2:C:373:LEU:HD12	1.69	0.58
1:G:374:ILE:H	1:G:374:ILE:CD1	2.17	0.58
1:D:252:LEU:O	1:D:256:VAL:HG13	2.03	0.58
1:H:7:LYS:HD2	1:H:38:GLY:O	2.03	0.58
1:B:73:LYS:HZ1	1:B:77:PRO:HD3	1.66	0.58
1:H:163:MET:HB2	1:H:170:VAL:CG2	2.34	0.58
1:H:63:GLN:HA	1:H:63:GLN:NE2	2.19	0.58
1:E:89:LEU:N	1:E:89:LEU:HD12	2.18	0.58
1:D:125:MET:HE3	1:D:134:MET:HB2	1.85	0.58
1:A:131:ALA:HA	1:A:134:MET:CE	2.33	0.58
1:G:309:ILE:HG23	1:G:318:VAL:HG22	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:HB2	1:D:107:PRO:HD3	1.84	0.58
1:D:25:LYS:HB3	1:D:340:LEU:HD11	1.84	0.58
1:H:125:MET:HA	1:H:125:MET:CE	2.34	0.58
1:D:308:LYS:HD2	1:D:309:ILE:O	2.04	0.58
1:D:106:ARG:H	1:D:106:ARG:HD2	1.67	0.58
1:H:113:THR:O	1:H:372:GLY:HA2	2.03	0.58
1:B:66:SER:HB2	1:B:67:GLN:OE1	2.04	0.58
1:H:120:TYR:CG	1:H:366:THR:CG2	2.86	0.58
1:D:99:HIS:CE1	1:D:123:GLU:HB3	2.39	0.58
1:E:176:LEU:HD23	1:E:199:MET:O	2.02	0.58
2:F:446:MET:CE	2:F:448:LEU:HD21	2.32	0.58
1:B:188:ILE:HG23	1:B:198:VAL:HG11	1.86	0.58
1:G:10:ARG:NH1	1:G:76:ARG:CZ	2.67	0.57
1:E:202:ASP:OD2	1:E:203:VAL:N	2.36	0.57
1:E:86:GLU:O	1:E:88:ALA:N	2.37	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
1:E:374:ILE:N	1:E:374:ILE:HD12	2.19	0.57
1:D:293:LEU:HD21	1:D:323:VAL:HG21	1.86	0.57
2:I:313:VAL:HB	2:I:388:VAL:HG22	1.86	0.57
2:C:371:PHE:HB2	2:C:376:ILE:HG12	1.85	0.57
1:E:106:ARG:HB3	1:E:107:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:ALA:HB3	1:E:264:THR:CG2	2.34	0.57
1:H:124:LEU:HD13	1:H:365:GLY:O	2.04	0.57
1:D:357:LYS:O	1:D:359:GLU:N	2.37	0.57
1:H:67:GLN:H	1:H:67:GLN:CD	2.07	0.57
1:B:100:LEU:C	1:B:102:ALA:N	2.55	0.57
1:G:180:VAL:HG21	1:G:211:VAL:HG21	1.86	0.57
1:G:10:ARG:NH1	1:G:76:ARG:NH2	2.51	0.57
1:D:179:GLY:HA2	5:D:400:NAD:H8A	1.85	0.57
1:G:160:PHE:N	1:G:161:PRO:HD2	2.19	0.57
1:G:34:ILE:CD1	1:G:56:THR:HB	2.34	0.57
1:E:183:ALA:HB3	1:E:264:THR:HG21	1.85	0.57
1:D:329:ALA:CB	1:E:158:ARG:HG3	2.33	0.57
1:B:136:ILE:HG13	1:B:137:LEU:N	2.18	0.57
1:E:16:VAL:O	1:E:18:ILE:N	2.38	0.57
1:H:309:ILE:HG12	1:H:318:VAL:HG13	1.85	0.57
1:D:60:THR:OG1	1:D:63:GLN:HG2	2.05	0.57
1:H:16:VAL:HG22	1:H:17:ALA:H	1.69	0.57
1:D:151:ASP:CG	1:D:326:ARG:HH21	2.08	0.57
1:G:273:PRO:HG3	5:G:400:NAD:C2A	2.34	0.57
1:B:67:GLN:O	1:B:67:GLN:HG2	2.05	0.57
1:D:4:ALA:HB1	1:D:34:ILE:O	2.04	0.57
1:G:282:THR:HG22	1:G:313:HIS:CD2	2.39	0.57
1:E:370:ARG:HH21	1:E:375:VAL:HG11	1.70	0.57
2:F:373:LEU:HD23	2:F:373:LEU:C	2.24	0.57
1:E:127:ARG:NH2	1:E:132:GLN:HG3	2.20	0.57
1:A:97:MET:HE3	1:A:343:LEU:HD12	1.85	0.57
1:H:346:HIS:NE2	1:H:362:THR:HG21	2.20	0.57
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.20	0.57
1:B:242:GLU:O	1:B:245:LYS:HB3	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
1:H:202:ASP:CG	5:H:400:NAD:H8A	2.25	0.57
1:D:221:VAL:CG1	1:D:250:ALA:HB3	2.34	0.57
2:C:414:ASP:HB3	2:C:417:LYS:HE3	1.87	0.57
2:F:437:ASN:HB3	2:F:440:PHE:CE2	2.40	0.57
1:A:69:ASP:O	1:A:95:VAL:HG23	2.05	0.57
1:H:282:THR:HG22	1:H:313:HIS:CD2	2.39	0.56
1:E:199:MET:CG	1:E:219:ILE:HD11	2.28	0.56
1:E:136:ILE:HD12	1:E:137:LEU:HD12	1.87	0.56
1:B:5:ILE:HG13	1:B:72:TRP:HB2	1.87	0.56
1:H:2:LYS:O	1:H:69:ASP:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:PHE:O	1:G:245:LYS:N	2.38	0.56
1:D:222:ASP:HB2	1:D:227:LYS:HE2	1.86	0.56
1:B:266:LEU:H	5:B:400:NAD:H52A	1.70	0.56
1:G:200:ALA:HB3	1:G:211:VAL:HG11	1.88	0.56
2:I:310:VAL:HG22	2:I:385:VAL:HB	1.86	0.56
1:H:243:PHE:C	1:H:245:LYS:H	2.08	0.56
1:H:312:LYS:HG3	1:H:313:HIS:CD2	2.40	0.56
2:I:439:LEU:C	2:I:441:PHE:H	2.08	0.56
2:I:440:PHE:HD2	2:I:447:MET:SD	2.28	0.56
1:E:125:MET:CE	1:E:134:MET:HB2	2.34	0.56
1:A:276:ILE:HA	1:A:280:MET:HE1	1.87	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
1:H:70:VAL:HG23	1:H:95:VAL:HB	1.87	0.56
2:F:450:GLY:HA3	2:F:455:MET:CE	2.35	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
1:H:73:LYS:HD2	1:H:75:GLN:O	2.05	0.56
1:E:250:ALA:O	1:E:253:LYS:HB3	2.05	0.56
1:D:50:LEU:C	1:D:55:ALA:HB3	2.25	0.56
1:B:96:LEU:HD23	1:B:112:LEU:CD2	2.36	0.56
2:I:304:MET:C	2:I:306:ASN:H	2.05	0.56
1:E:143:LEU:HD12	1:E:331:ALA:HB2	1.86	0.56
1:A:80:ALA:HA	1:A:85:ASP:HB2	1.87	0.56
1:H:124:LEU:O	1:H:125:MET:C	2.44	0.56
1:B:137:LEU:H	1:B:137:LEU:HD12	1.71	0.56
1:G:118:THR:CB	1:G:370:ARG:HA	2.35	0.56
1:D:208:LYS:HD2	1:D:209:GLU:N	2.20	0.56
1:E:362:THR:CG2	1:E:363:VAL:H	2.18	0.56
1:B:190:THR:HA	1:B:193:ARG:HD2	1.87	0.56
1:E:264:THR:O	1:E:264:THR:HG22	2.04	0.56
1:D:281:VAL:O	1:D:281:VAL:HG12	2.04	0.56
1:H:116:LYS:HA	1:H:372:GLY:H	1.69	0.56
1:H:265:ALA:HB3	1:H:300:ASN:OD1	2.04	0.56
1:D:35:VAL:HG21	1:D:50:LEU:HD23	1.87	0.56
1:E:128:ILE:HG13	1:E:128:ILE:O	2.04	0.56
1:G:199:MET:CE	1:G:217:LYS:HB2	2.35	0.56
1:D:351:THR:O	1:D:353:THR:HG22	2.06	0.56
1:H:179:GLY:O	1:H:181:GLY:N	2.39	0.56
1:D:342:PHE:CE1	1:D:362:THR:O	2.58	0.56
1:G:342:PHE:HE1	1:G:362:THR:HG23	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:182:VAL:HG13	1:H:183:ALA:H	1.70	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:D:68:ALA:O	1:D:91:LYS:CG	2.54	0.56
1:H:202:ASP:HA	5:H:400:NAD:C8A	2.35	0.56
2:I:393:ASP:OD1	2:I:431:GLY:HA3	2.05	0.56
1:B:354:LEU:HD11	1:B:356:MET:SD	2.46	0.56
1:G:274:VAL:HG13	1:G:302:PRO:HD3	1.88	0.56
2:I:452:ALA:H	6:I:500:NDP:C2A	2.19	0.56
1:D:285:LYS:HZ1	1:E:44:SER:HB3	1.70	0.56
1:G:281:VAL:O	1:G:281:VAL:HG12	2.06	0.56
1:B:87:VAL:HG13	1:B:88:ALA:N	2.21	0.56
1:H:72:TRP:CE3	1:H:339:LEU:HB3	2.40	0.56
1:D:221:VAL:HG21	1:D:247:GLN:HA	1.88	0.56
2:F:410:MET:HG3	2:F:411:PRO:HD2	1.88	0.56
1:B:66:SER:O	1:B:91:LYS:HB2	2.06	0.56
1:H:18:ILE:HG12	1:H:19:SER:N	2.21	0.55
1:A:270:LYS:CB	1:A:271:PRO:CD	2.78	0.55
1:D:2:LYS:HD2	1:D:32:GLU:CB	2.35	0.55
2:I:451:ASP:O	2:I:452:ALA:C	2.44	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:B:291:ILE:HD13	1:B:318:VAL:HB	1.88	0.55
2:C:346:HIS:CD2	2:C:373:LEU:HD12	2.41	0.55
1:G:164:MET:CE	2:I:370:VAL:HG12	2.36	0.55
1:G:164:MET:HE1	2:I:370:VAL:HG12	1.88	0.55
2:I:298:GLU:N	2:I:298:GLU:OE2	2.37	0.55
1:H:74:VAL:CG2	1:H:75:GLN:H	2.12	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:A:2:LYS:HB3	1:A:68:ALA:HA	1.88	0.55
1:H:47:ASP:CB	1:H:57:ILE:HD11	2.35	0.55
1:H:295:VAL:O	1:H:295:VAL:HG22	2.06	0.55
1:G:376:HIS:CD2	1:G:378:ALA:HB2	2.40	0.55
1:H:92:GLU:HB2	1:H:116:LYS:NZ	2.21	0.55
1:B:76:ARG:HB3	1:B:100:LEU:HA	1.88	0.55
1:A:149:VAL:HG11	1:A:190:THR:HG22	1.89	0.55
1:H:181:GLY:O	1:H:185:LEU:HD12	2.06	0.55
1:H:33:VAL:O	1:H:34:ILE:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:TYR:HB3	1:B:366:THR:HG21	1.88	0.55
2:F:455:MET:O	2:F:459:ILE:HG13	2.06	0.55
1:H:156:PHE:CE2	1:H:158:ARG:HB2	2.41	0.55
1:D:223:ASP:HB3	1:D:228:THR:HG21	1.89	0.55
1:G:326:ARG:NH2	1:G:326:ARG:HG2	2.22	0.55
1:G:326:ARG:O	3:H:600:SUC:O4'	2.25	0.55
1:E:2:LYS:HD3	1:E:32:GLU:CB	2.36	0.55
1:H:8:GLU:H	1:H:8:GLU:CD	2.09	0.55
1:D:26:LEU:HD11	1:D:72:TRP:CZ3	2.42	0.55
1:D:34:ILE:HG23	1:D:56:THR:O	2.07	0.55
1:G:106:ARG:N	1:G:107:PRO:CD	2.69	0.55
1:A:194:LEU:HD21	1:B:194:LEU:HG	1.88	0.55
1:G:111:ALA:HA	1:G:114:LYS:HG3	1.88	0.55
1:E:108:VAL:O	1:E:112:LEU:HD12	2.07	0.55
1:G:280:MET:C	1:G:282:THR:H	2.10	0.55
1:E:284:MET:HE2	1:E:290:ILE:HD11	1.89	0.54
1:G:23:VAL:HG11	1:G:55:ALA:HB2	1.89	0.54
2:I:403:PRO:HG3	2:I:408:TYR:CZ	2.42	0.54
1:D:29:LEU:HD22	1:D:347:VAL:HG11	1.90	0.54
1:D:344:THR:HA	1:D:347:VAL:HG23	1.88	0.54
1:D:357:LYS:C	1:D:359:GLU:H	2.10	0.54
1:E:9:ARG:O	1:E:10:ARG:C	2.45	0.54
1:D:18:ILE:C	1:D:18:ILE:HD13	2.28	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:C:315:GLY:HA3	2:C:391:ALA:HB2	1.89	0.54
2:I:371:PHE:HB2	2:I:376:ILE:HB	1.89	0.54
1:H:8:GLU:HG3	1:H:73:LYS:HE2	1.89	0.54
1:H:277:THR:OG1	1:H:280:MET:HG3	2.08	0.54
1:D:32:GLU:O	1:D:34:ILE:HD12	2.07	0.54
2:I:422:LEU:HD12	2:I:446:MET:HB3	1.88	0.54
1:H:25:LYS:CE	1:H:25:LYS:HA	2.37	0.54
2:C:324:GLN:HB2	2:C:363:ALA:HB2	1.89	0.54
1:G:182:VAL:HG12	5:G:400:NAD:O1N	2.07	0.54
1:A:375:VAL:CG2	1:A:375:VAL:O	2.55	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:H:300:ASN:N	1:H:300:ASN:HD22	2.06	0.54
2:C:399:ALA:HA	2:C:408:TYR:HA	1.90	0.54
1:H:15:ARG:CG	1:H:15:ARG:HH21	2.19	0.54
2:I:330:MET:HG3	2:I:463:MET:CE	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:ASP:CB	1:H:207:THR:HG21	2.38	0.54
1:B:118:THR:HA	1:B:370:ARG:HA	1.90	0.54
1:E:303:LEU:H	1:E:303:LEU:HD12	1.73	0.54
1:A:277:THR:O	1:A:279:GLU:N	2.41	0.54
1:D:2:LYS:NZ	1:D:32:GLU:HG2	2.23	0.54
2:I:422:LEU:HG	2:I:448:LEU:CD1	2.35	0.54
1:A:380:THR:HG22	1:A:380:THR:O	2.08	0.54
1:D:205:ALA:C	1:D:207:THR:H	2.11	0.54
1:D:164:MET:HG3	2:F:345:ILE:HG21	1.89	0.54
1:A:180:VAL:HG21	1:A:207:THR:HG21	1.88	0.54
1:B:370:ARG:HH12	1:B:375:VAL:HG11	1.72	0.54
1:D:10:ARG:HG3	1:D:10:ARG:NH2	2.21	0.54
1:D:164:MET:HG2	2:F:357:ASN:ND2	2.22	0.54
1:E:121:ALA:HB1	1:E:123:GLU:CD	2.28	0.54
1:A:147:ARG:HG3	1:A:151:ASP:OD2	2.07	0.54
1:D:294:ALA:O	1:D:299:GLY:N	2.41	0.54
1:D:4:ALA:HB2	1:D:34:ILE:HB	1.90	0.54
1:A:21:GLU:CD	1:A:21:GLU:H	2.10	0.54
2:I:309:LYS:O	2:I:384:ASP:HB2	2.08	0.54
2:C:330:MET:HG2	2:C:334:LEU:CD2	2.38	0.54
1:A:97:MET:CE	1:A:343:LEU:HD12	2.38	0.54
1:D:193:ARG:HB3	1:E:193:ARG:O	2.07	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:B:5:ILE:HG23	1:B:17:ALA:HB3	1.89	0.54
1:A:360:ASP:OD2	1:A:362:THR:HB	2.08	0.54
1:E:369:THR:O	1:E:369:THR:HG23	2.06	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
2:F:348:VAL:HG21	2:F:410:MET:CE	2.37	0.54
1:B:379:LEU:HD12	1:B:379:LEU:N	2.23	0.54
2:C:321:ALA:O	2:C:322:GLN:HB2	2.08	0.54
1:B:204:ARG:HH21	1:B:207:THR:HG22	1.73	0.54
1:A:354:LEU:HD11	1:A:356:MET:HE1	1.90	0.53
1:H:203:VAL:HG12	1:H:243:PHE:CZ	2.44	0.53
1:B:128:ILE:HG12	1:B:131:ALA:CB	2.37	0.53
1:G:62:ALA:HB2	1:G:89:LEU:CD2	2.37	0.53
1:B:244:ARG:HA	1:B:247:GLN:HB3	1.90	0.53
1:A:80:ALA:CA	1:A:85:ASP:HB2	2.38	0.53
1:H:7:LYS:HB2	1:H:39:ALA:CA	2.38	0.53
1:E:108:VAL:O	1:E:111:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLU:C	1:E:88:ALA:N	2.61	0.53
1:B:199:MET:HE2	1:B:217:LYS:HB3	1.89	0.53
2:I:395:THR:HB	2:I:415:VAL:HG21	1.89	0.53
1:H:214:LEU:HD11	2:I:352:MET:SD	2.49	0.53
1:B:106:ARG:HB3	1:B:107:PRO:HD3	1.90	0.53
1:D:164:MET:CG	2:F:357:ASN:HD21	2.21	0.53
2:C:379:SER:O	2:C:382:THR:N	2.41	0.53
1:E:58:ALA:CB	1:E:64:ALA:HA	2.38	0.53
1:A:140:GLN:C	1:A:142:ASN:H	2.11	0.53
2:C:321:ALA:HB3	2:C:452:ALA:HB3	1.90	0.53
1:B:100:LEU:O	1:B:102:ALA:N	2.42	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:N	1:B:137:LEU:HD12	2.24	0.53
1:D:293:LEU:HD23	1:D:323:VAL:HG21	1.91	0.53
1:G:284:MET:HG3	1:G:315:VAL:HG21	1.90	0.53
1:H:7:LYS:O	1:H:9:ARG:HD2	2.09	0.53
1:H:112:LEU:CD1	1:H:112:LEU:N	2.71	0.53
1:G:62:ALA:CA	1:G:89:LEU:HD23	2.38	0.53
1:A:265:ALA:CB	1:A:275:LEU:HD11	2.39	0.53
1:D:6:PRO:HD2	1:D:72:TRP:O	2.08	0.53
1:E:5:ILE:HD12	1:E:5:ILE:N	2.24	0.53
1:H:38:GLY:H	1:H:47:ASP:CG	2.12	0.53
1:H:203:VAL:H	5: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
1:D:8:GLU:HB3	1:D:13:GLU:HB3	1.91	0.53
1:G:203:VAL:CG2	1:G:204:ARG:H	2.18	0.53
1:A:327:VAL:O	1:A:327:VAL:HG12	2.08	0.53
1:G:95:VAL:HG22	1:G:118:THR:HG23	1.90	0.53
1:E:344:THR:O	1:E:347:VAL:HG12	2.08	0.53
2:I:463:MET:O	2:I:464:ASN:HB2	2.09	0.53
1:B:190:THR:HA	1:B:193:ARG:CD	2.39	0.53
2:F:346:HIS:HB3	2:F:349:ALA:HB2	1.90	0.53
1:A:113:THR:HG22	1:A:114:LYS:N	2.24	0.53
1:G:128:ILE:HD12	1:G:129:SER:N	2.23	0.53
1:G:62:ALA:CB	1:G:89:LEU:HD23	2.37	0.53
1:A:327:VAL:HG12	1:A:330:ASP:HB2	1.91	0.53
1:D:202:ASP:OD1	1:D:203:VAL:N	2.41	0.53
2:C:420:THR:HB	1:H:162:MET:HE1	1.91	0.53
1:E:214:LEU:HD21	2:F:355:HIS:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:374:GLU:H	2:F:374:GLU:CD	2.11	0.53
1:D:123:GLU:HG2	1:D:124:LEU:HD13	1.89	0.53
2:F:445:THR:HG22	2:F:446:MET:N	2.24	0.53
1:G:22:VAL:HG13	1:G:340:LEU:HD12	1.91	0.53
2:I:331:ALA:O	2:I:335:LYS:HD3	2.09	0.53
1:D:122:MET:C	1:D:124:LEU:H	2.11	0.53
1:D:8:GLU:OE1	1:D:75:GLN:N	2.40	0.53
2:C:392:ASN:HB3	6:C:500:NDP:O1A	2.09	0.53
1:D:244:ARG:N	1:D:244:ARG:HD3	2.24	0.53
2:I:451:ASP:H	2:I:454:LYS:HE2	1.73	0.53
1:B:100:LEU:C	1:B:102:ALA:H	2.13	0.53
1:B:71:VAL:HG12	1:B:96:LEU:HA	1.90	0.53
1:H:176:LEU:HA	1:H:199:MET:O	2.09	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:B:272:ALA:HB1	1:B:300:ASN:HD21	1.74	0.53
1:B:5:ILE:HD13	1:B:18:ILE:HD12	1.91	0.52
1:D:267:ILE:O	1:D:268:PRO:O	2.27	0.52
1:A:277:THR:N	1:A:280:MET:HE3	2.24	0.52
1:G:153:ALA:HA	1:G:160:PHE:CE1	2.44	0.52
2:F:416:GLU:HG3	2:F:439:LEU:HD11	1.91	0.52
1:B:265:ALA:HB3	1:B:275:LEU:HD11	1.90	0.52
1:E:3:ILE:O	1:E:3:ILE:HG23	2.08	0.52
1:G:78:MET:N	1:G:86:GLU:HB2	2.23	0.52
1:E:312:LYS:O	1:E:313:HIS:HB2	2.09	0.52
1:B:1:MET:HE2	1:B:353:THR:HA	1.91	0.52
1:E:2:LYS:HD3	1:E:32:GLU:HB2	1.90	0.52
1:H:103:LEU:HD12	1:H:103:LEU:N	2.23	0.52
1:H:330:ASP:C	1:H:333:PRO:HD2	2.29	0.52
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:H:85:ASP:OD2	1:H:88:ALA:HB3	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:D:342:PHE:C	1:D:345:PRO:HD2	2.29	0.52
1:D:3:ILE:HG22	1:D:31:PHE:HB3	1.90	0.52
1:D:265:ALA:HB3	1:D:300:ASN:ND2	2.24	0.52
1:D:327:VAL:O	1:D:329:ALA:N	2.43	0.52
1:H:294:ALA:C	1:H:296:GLU:H	2.12	0.52
1:B:273:PRO:HG3	5:B:400:NAD:N6A	2.24	0.52
1:H:122:MET:C	1:H:124:LEU:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:136:ILE:HD12	1:E:136:ILE:C	2.30	0.52
2:F:374:GLU:OE1	2:F:374:GLU:N	2.42	0.52
1:E:252:LEU:O	1:E:256:VAL:HG22	2.10	0.52
1:G:370:ARG:O	1:G:371:ASP:C	2.46	0.52
1:E:180:VAL:O	1:E:180:VAL:HG12	2.09	0.52
2:F:450:GLY:HA3	2:F:455:MET:HE3	1.92	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:291:ILE:HD13	1:E:318:VAL:HB	1.91	0.52
1:H:277:THR:O	1:H:281:VAL:HG13	2.10	0.52
1:A:46:THR:HG23	1:A:49:ALA:CB	2.30	0.52
2:I:333:VAL:O	2:I:336:LYS:HG2	2.09	0.52
1:H:340:LEU:CD1	1:H:344:THR:HG23	2.38	0.52
2:C:456:THR:O	2:C:460:VAL:HG23	2.10	0.52
2:I:319:ALA:HA	2:I:359:LEU:HD13	1.92	0.52
1:E:264:THR:CG2	1:E:264:THR:O	2.57	0.52
1:A:85:ASP:OD2	1:A:88:ALA:HB2	2.09	0.52
1:B:78:MET:HG3	1:B:86:GLU:OE1	2.10	0.52
1:H:98:CYS:N	1:H:122:MET:HE1	2.25	0.52
1:A:355:VAL:HG13	1:A:355:VAL:O	2.10	0.52
1:B:368:VAL:CG1	1:B:379:LEU:HD22	2.40	0.52
2:I:324:GLN:HG2	2:I:325:HIS:H	1.75	0.52
2:F:459:ILE:O	2:F:463:MET:HG3	2.10	0.52
1:A:207:THR:HG22	1:A:218:PHE:CE1	2.42	0.52
1:E:260:ILE:HG12	1:E:289:VAL:CG1	2.40	0.52
1:G:7:LYS:HG3	1:G:39:ALA:HA	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
2:C:346:HIS:CD2	2:C:347:PRO:HD2	2.45	0.52
1:A:275:LEU:O	1:A:280:MET:HE1	2.10	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:A:370:ARG:HD2	1:A:375:VAL:HG11	1.92	0.52
1:H:147:ARG:HG3	1:H:327:VAL:HG22	1.92	0.52
2:I:453:LYS:HE2	2:I:457:GLU:CD	2.31	0.52
2:I:336:LYS:HG3	2:I:337:GLU:H	1.75	0.52
1:D:323:VAL:HB	1:D:324:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:GLN:HG2	5:G:400:NAD:O7N	2.10	0.52
1:E:207:THR:HG22	1:E:218:PHE:CE2	2.44	0.52
2:C:309:LYS:HZ1	2:C:382:THR:HB	1.74	0.52
1:B:184:GLY:O	1:B:187:ALA:HB3	2.10	0.52
1:B:242:GLU:HA	1:B:242:GLU:OE2	2.10	0.52
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
1:B:370:ARG:NH1	1:B:375:VAL:HG11	2.24	0.51
1:A:277:THR:C	1:A:279:GLU:N	2.64	0.51
1:A:262:ILE:HD13	1:A:291:ILE:HB	1.91	0.51
1:A:374:ILE:HB	1:A:380:THR:HG21	1.92	0.51
1:E:120:TYR:OH	1:E:356:MET:HG3	2.10	0.51
1:A:115:ARG:O	1:A:116:LYS:HB2	2.10	0.51
1:A:305:GLU:HB3	1:A:308:LYS:HD2	1.92	0.51
2:F:424:ILE:O	2:F:424:ILE:HG22	2.09	0.51
2:I:317:GLY:HA3	2:I:390:GLY:HA3	1.92	0.51
1:D:282:THR:O	1:D:282:THR:HG22	2.11	0.51
1:G:203:VAL:CG2	1:G:204:ARG:N	2.69	0.51
1:E:320:HIS:CE1	1:E:326:ARG:NH2	2.79	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:H:103:LEU:HD11	1:H:124:LEU:HD21	1.91	0.51
1:H:125:MET:HA	1:H:125:MET:HE2	1.92	0.51
1:H:128:ILE:O	1:H:132:GLN:CG	2.58	0.51
2:F:407:ILE:O	2:F:408:TYR:C	2.49	0.51
2:I:432:TYR:C	2:I:434:GLY:N	2.64	0.51
1:H:96:LEU:HD23	1:H:96:LEU:C	2.30	0.51
1:G:208:LYS:O	1:G:212:GLU:HG3	2.09	0.51
2:I:304:MET:C	2:I:306:ASN:N	2.63	0.51
2:I:380:PHE:CZ	2:I:413:LEU:HD22	2.44	0.51
1:A:80:ALA:HB2	1:A:85:ASP:HB2	1.91	0.51
1:E:252:LEU:HG	1:E:252:LEU:O	2.08	0.51
1:A:222:ASP:OD2	1:A:222:ASP:N	2.44	0.51
1:D:3:ILE:CB	1:D:70:VAL:HG23	2.41	0.51
1:E:125:MET:CE	1:E:342:PHE:HD2	2.20	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:D:7:LYS:O	1:D:9:ARG:HG3	2.11	0.51
1:B:244:ARG:CD	1:B:244:ARG:H	2.24	0.51
1:G:176:LEU:HD23	1:G:199:MET:O	2.11	0.51
1:E:266:LEU:HD13	1:E:294:ALA:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LEU:HD23	1:D:89:LEU:O	2.11	0.51
1:H:368:VAL:HG13	1:H:376:HIS:HB3	1.93	0.51
1:H:202:ASP:CA	5:H:400:NAD:H8A	2.39	0.51
2:F:432:TYR:CD2	6:F:500:NDP:C1D	2.84	0.51
2:I:445:THR:HG22	2:I:447:MET:HE2	1.93	0.51
1:D:248:ALA:HA	1:D:251:VAL:CG2	2.40	0.51
1:D:267:ILE:HD11	5:D:400:NAD:H2A	1.93	0.51
1:H:266:LEU:HD12	1:H:272:ALA:HB2	1.92	0.51
1:A:211:VAL:HG12	1:A:212:GLU:N	2.25	0.51
1:D:91:LYS:HG3	1:D:91:LYS:O	2.11	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: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:D:275:LEU:CD1	1:D:300:ASN:HD22	2.13	0.51
1:D:160:PHE:N	1:D:161:PRO:HD2	2.26	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:113:THR:CG2	1:G:373:ALA:HA	2.41	0.51
1:G:13:GLU:OE2	1:G:15:ARG:HB2	2.11	0.51
1:G:133:SER:O	1:G:338:ASN:HA	2.11	0.51
2:I:336:LYS:CG	2:I:337:GLU:N	2.72	0.51
1:D:136:ILE:HG22	1:D:338:ASN:CB	2.39	0.51
1:H:266:LEU:HD13	1:H:294:ALA:HB2	1.92	0.51
1:H:182:VAL:CG1	1:H:183:ALA:N	2.74	0.51
2:C:309:LYS:HZ3	2:C:382:THR:HB	1.76	0.51
1:G:154:TYR:O	1:H:147:ARG:NH2	2.36	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:A:160:PHE:O	1:A:172:PRO:HA	2.11	0.51
1:D:304:SER:O	1:D:305:GLU:HG2	2.11	0.51
2:F:412:ILE:HD12	2:F:412:ILE:O	2.11	0.51
1:H:112:LEU:O	1:H:115:ARG:HB2	2.11	0.51
1:H:61:ALA:O	1:H:65:LEU:HD22	2.11	0.51
1:E:7:LYS:HB2	1:E:39:ALA:HA	1.92	0.51
2:I:389:ILE:O	2:I:389:ILE:HG23	2.10	0.51
1:A:17:ALA:HB2	1:A:74:VAL:HG22	1.92	0.51
1:B:22:VAL:HG21	1:B:336:ALA:CB	2.41	0.50
1:H:129:SER:C	1:H:132:GLN:HG3	2.31	0.50
1:H:357:LYS:HB3	1:H:360:ASP:CB	2.34	0.50
2:F:432:TYR:HD2	6:F:500:NDP:H1D	1.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:ILE:O	1:G:130:ARG:N	2.44	0.50
1:D:267:ILE:O	1:D:267:ILE:HG22	2.10	0.50
2:C:413:LEU:O	2:C:415:VAL:N	2.43	0.50
1:B:74:VAL:HG23	1:B:75:GLN:N	2.26	0.50
1:H:29:LEU:CD2	1:H:344:THR:HG22	2.41	0.50
1:B:281:VAL:HA	1:B:284:MET:HE3	1.93	0.50
1:B:188:ILE:HA	1:B:198:VAL:HG11	1.93	0.50
2:I:433:ALA:C	2:I:435:VAL:H	2.14	0.50
1:E:270:LYS:N	1:E:270:LYS:HE3	2.26	0.50
1:B:3:ILE:HG13	1:B:70:VAL:CG1	2.41	0.50
1:E:279:GLU:O	1:E:282:THR:OG1	2.20	0.50
1:A:273:PRO:O	1:A:300:ASN:HA	2.10	0.50
1:H:65:LEU:N	1:H:65:LEU:HD12	2.26	0.50
1:B:98:CYS:SG	1:B:100:LEU:HG	2.52	0.50
2:I:324:GLN:HG2	2:I:325:HIS:N	2.26	0.50
1:E:212:GLU:C	1:E:214:LEU:N	2.63	0.50
1:H:179:GLY:HA3	1:H:264:THR:OG1	2.12	0.50
1:G:89:LEU:N	1:G:89:LEU:HD12	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:D:5:ILE:N	1:D:34:ILE:O	2.41	0.50
1:D:16:VAL:HG11	1:D:40:GLY:HA3	1.91	0.50
1:D:252:LEU:C	1:D:254:GLU:H	2.13	0.50
1:G:22:VAL:HG13	1:G:340:LEU:CD1	2.41	0.50
1:D:7:LYS:HB2	1:D:39:ALA:HA	1.92	0.50
2:I:328:ARG:HD2	2:I:328:ARG:O	2.11	0.50
1:A:313:HIS:O	1:A:315:VAL:HG23	2.11	0.50
1:D:97:MET:HB2	1:D:122:MET:HE2	1.94	0.50
1:E:176:LEU:HA	1:E:199:MET:O	2.12	0.50
1:D:23:VAL:O	1:D:26:LEU:N	2.42	0.50
1:D:5:ILE:O	1:D:35:VAL:HA	2.11	0.50
1:D:291:ILE:CD1	1:D:291:ILE:N	2.74	0.50
1:B:5:ILE:HB	1:B:35:VAL:HG12	1.94	0.50
1:D:343:LEU:HG	1:D:354:LEU:HD12	1.93	0.50
1:D:74:VAL:HG12	1:D:75:GLN:N	2.26	0.50
1:D:68:ALA:C	1:D:91:LYS:HD3	2.29	0.50
1:H:180:VAL:HG21	1:H:211:VAL:CG2	2.41	0.50
1:G:86:GLU:HA	1:G:89:LEU:HD13	1.92	0.50
1:D:23:VAL:CG1	1:D:55:ALA:HB2	2.39	0.50
1:B:134:MET:HG2	1:B:342:PHE:H	1.75	0.50
1:D:285:LYS:HD3	1:D:286:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:HA	1:B:199:MET:O	2.12	0.50
1:E:374:ILE:H	1:E:374:ILE:CD1	2.24	0.50
1:G:208:LYS:NZ	1:G:220:THR:HG23	2.27	0.50
1:G:199:MET:HE1	1:G:217:LYS:HB2	1.93	0.50
1:E:266:LEU:CD1	1:E:294:ALA:HA	2.42	0.50
1:G:299:GLY:C	1:G:301:CYS:H	2.15	0.50
1:H:103:LEU:CD1	1:H:103:LEU:H	2.23	0.50
1:G:78:MET:H	1:G:86:GLU:CB	2.24	0.50
1:D:294:ALA:CB	1:D:300:ASN:OD1	2.58	0.50
1:G:97:MET:HE1	1:G:343:LEU:HD13	1.93	0.50
1:D:376:HIS:CD2	1:D:378:ALA:HB2	2.46	0.50
1:H:182:VAL:CG1	1:H:183:ALA:H	2.25	0.50
1:D:252:LEU:HD23	1:D:252:LEU:C	2.32	0.50
1:E:105:ASN:O	1:E:109:VAL:HG23	2.12	0.50
1:H:297:ALA:C	1:H:299:GLY:H	2.15	0.50
1:B:29:LEU:HD21	1:B:344:THR:HB	1.93	0.50
1:H:243:PHE:O	1:H:245:LYS:N	2.40	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:113:THR:HG23	1:H:369:THR:OG1	2.12	0.50
1:H:360:ASP:O	1:H:362:THR:N	2.45	0.50
1:E:282:THR:HG22	1:E:313:HIS:CE1	2.47	0.50
1:H:311:VAL:HG23	1:H:315:VAL:O	2.12	0.50
1:G:380:THR:HG23	1:G:380:THR:O	2.12	0.49
1:D:78:MET:HB2	1:D:86:GLU:HG3	1.92	0.49
2:F:437:ASN:HB3	2:F:440:PHE:CZ	2.47	0.49
1:A:74:VAL:HA	1:A:335:PHE:CE2	2.47	0.49
1:E:172:PRO:HG3	2:I:443:ASN:O	2.12	0.49
1:H:58:ALA:CB	1:H:64:ALA:HA	2.42	0.49
1:D:46:THR:O	1:D:50:LEU:HD12	2.12	0.49
1:G:160:PHE:CZ	1:G:260:ILE:HD12	2.47	0.49
1:E:360:ASP:OD1	1:E:362:THR:HG22	2.12	0.49
1:B:156:PHE:CZ	1:B:259:ASP:HB3	2.47	0.49
1:G:291:ILE:O	1:G:291:ILE:HG22	2.10	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:D:360:ASP:CG	1:D:362:THR:HB	2.33	0.49
1:G:360:ASP:OD1	1:G:362:THR:HB	2.12	0.49
1:G:158:ARG:HB2	1:H:330:ASP:HB2	1.95	0.49
1:E:366:THR:O	1:E:366:THR:HG22	2.11	0.49
2:I:337:GLU:HG3	2:I:337:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:VAL:HG11	1:E:211:VAL:HG22	1.95	0.49
1:D:1:MET:SD	1:D:353:THR:HA	2.52	0.49
1:E:272:ALA:CB	1:E:299:GLY:H	2.25	0.49
1:A:223:ASP:OD2	1:A:243:PHE:HZ	1.95	0.49
1:B:18:ILE:HG12	1:B:19:SER:H	1.77	0.49
1:H:292:ASP:HB3	1:H:295:VAL:HB	1.94	0.49
1:E:200:ALA:O	1:E:219:ILE:HG12	2.12	0.49
1:E:128:ILE:HD11	1:E:130:ARG:NH2	2.26	0.49
1:H:266:LEU:HD12	1:H:272:ALA:CB	2.42	0.49
1:E:370:ARG:HB2	1:E:375:VAL:HG21	1.94	0.49
1:B:344:THR:HA	1:B:347:VAL:HG12	1.95	0.49
1:H:51:THR:HG23	1:H:55:ALA:O	2.13	0.49
1:H:61:ALA:C	1:H:65:LEU:HD13	2.32	0.49
1:D:199:MET:CG	1:D:219:ILE:HD11	2.43	0.49
1:G:57:ILE:HG22	1:G:57:ILE:O	2.11	0.49
1:D:334:LEU:HD22	1:E:167:ALA:CB	2.43	0.49
1:H:135:ASP:OD2	1:H:135:ASP:C	2.50	0.49
1:B:343:LEU:HD23	1:B:344:THR:N	2.28	0.49
1:A:354:LEU:HG	1:A:355:VAL:N	2.28	0.49
2:F:401:THR:O	2:F:403:PRO:CD	2.52	0.49
1:G:248:ALA:HB1	1:G:280:MET:CE	2.42	0.49
1:A:163:MET:HE3	1:A:170:VAL:HG11	1.95	0.49
1:B:178:PHE:HB3	1:B:275:LEU:HD13	1.95	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:295:VAL:HG13	1:A:296:GLU:N	2.28	0.49
1:H:115:ARG:O	1:H:116:LYS:HB2	2.13	0.49
1:H:357:LYS:C	1:H:359:GLU:H	2.16	0.49
1:D:344:THR:HA	1:D:347:VAL:CG2	2.43	0.49
1:D:118:THR:HG23	1:D:370:ARG:HG3	1.95	0.49
1:D:95:VAL:HG22	1:D:118:THR:HB	1.93	0.49
1:G:10:ARG:NH2	1:G:78:MET:HG3	2.27	0.49
1:D:330:ASP:CG	1:E:158:ARG:HG2	2.33	0.49
2:C:350:GLY:C	6:C:500:NDP:H71N	2.16	0.49
1:E:164:MET:SD	2:I:446:MET:HE1	2.53	0.49
1:D:224:GLU:H	1:D:227:LYS:HG2	1.78	0.49
1:B:100:LEU:HD12	1:B:121:ALA:HA	1.95	0.49
1:H:348:ASP:N	1:H:353:THR:O	2.43	0.49
1:B:181:GLY:HA3	5:B:400:NAD:O1N	2.13	0.49
1:B:339:LEU:O	1:B:340:LEU:C	2.50	0.49
1:D:343:LEU:HD23	1:D:343:LEU:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:LYS:HE3	1:G:75:GLN:O	2.13	0.49
1:G:72:TRP:NE1	1:G:97:MET:HE1	2.17	0.49
2:I:451:ASP:O	2:I:454:LYS:N	2.45	0.49
1:G:26:LEU:O	1:G:31:PHE:HB2	2.12	0.49
2:I:402:ASP:O	2:I:408:TYR:HB2	2.13	0.49
1:B:19:SER:HB3	1:B:22:VAL:CG2	2.42	0.49
1:H:119:ALA:H	1:H:369:THR:CG2	2.26	0.49
1:A:265:ALA:HB2	1:A:275:LEU:HD11	1.95	0.49
1:H:25:LYS:HA	1:H:25:LYS:HE3	1.94	0.49
1:A:103:LEU:HD21	1:A:124:LEU:HD11	1.94	0.49
1:G:244:ARG:HG2	1:G:244:ARG:O	2.13	0.49
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:B:128:ILE:HG12	1:B:131:ALA:HB3	1.95	0.48
1:G:279:GLU:O	1:G:283:LYS:HG2	2.13	0.48
1:E:122:MET:CE	1:E:339:LEU:HG	2.43	0.48
2:F:305:LYS:HZ2	2:F:337:GLU:HG3	1.77	0.48
1:A:363:VAL:O	1:A:363:VAL:HG12	2.13	0.48
1:D:97:MET:O	1:D:98:CYS:HB3	2.13	0.48
1:G:130:ARG:NH1	1:G:360:ASP:OD1	2.45	0.48
1:B:113:THR:HG23	1:B:372:GLY:O	2.14	0.48
1:A:305:GLU:HB2	1:A:310:VAL:HG21	1.96	0.48
1:D:105:ASN:O	1:D:109:VAL:HG13	2.13	0.48
1:D:108:VAL:HG13	1:D:109:VAL:N	2.27	0.48
1:A:17:ALA:HB2	1:A:74:VAL:CG2	2.43	0.48
2:I:435:VAL:HG22	2:I:436:GLU:N	2.28	0.48
1:B:341:ASN:O	1:B:343:LEU:N	2.45	0.48
1:A:362:THR:HG22	1:A:363:VAL:N	2.28	0.48
1:H:276:ILE:HA	1:H:280:MET:SD	2.53	0.48
1:D:354:LEU:C	1:D:354:LEU:HD23	2.32	0.48
2:F:407:ILE:O	2:F:408:TYR:O	2.31	0.48
1:E:10:ARG:NH2	1:E:76:ARG:HG3	2.27	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:A:163:MET:CE	1:A:170:VAL:HG11	2.43	0.48
1:H:27:VAL:HA	1:H:31:PHE:O	2.14	0.48
1:E:169:THR:OG1	2:I:303:ILE:HG12	2.12	0.48
1:A:80:ALA:CB	1:A:85:ASP:HB2	2.42	0.48
1:D:311:VAL:HA	1:D:315:VAL:O	2.13	0.48
1:D:85:ASP:OD2	1:D:88:ALA:HB3	2.14	0.48
1:H:10:ARG:HH11	1:H:76:ARG:HE	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:LEU:HD23	1:D:347:VAL:CG2	2.43	0.48
2:I:437:ASN:C	2:I:439:LEU:H	2.17	0.48
1:D:239:MET:H	1:D:244:ARG:HH11	1.59	0.48
2:I:316:TYR:CD1	2:I:351:ARG:HG2	2.49	0.48
1:D:134:MET:CE	1:D:341:ASN:O	2.61	0.48
1:A:138:SER:C	1:A:140:GLN:H	2.16	0.48
2:I:435:VAL:HG22	2:I:436:GLU:O	2.14	0.48
1:B:85:ASP:OD1	1:B:88:ALA:HB3	2.13	0.48
2:I:439:LEU:O	2:I:441:PHE:N	2.47	0.48
2:C:425:LYS:CB	2:C:425:LYS:HZ3	2.27	0.48
1:D:239:MET:HB2	1:D:244:ARG:NE	2.19	0.48
1:D:223:ASP:HA	1:D:227:LYS:HG2	1.95	0.48
1:B:267:ILE:HD11	5:B:400:NAD:N1A	2.29	0.48
1:B:90:ILE:O	1:B:91:LYS:C	2.50	0.48
1:G:332:SER:HB2	1:G:333:PRO:HD3	1.95	0.48
2:C:308:SER:HB2	2:C:384:ASP:OD2	2.14	0.48
1:G:96:LEU:HB3	1:G:119:ALA:HB2	1.95	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:H:98:CYS:O	1:H:121:ALA:HA	2.13	0.48
1:H:121:ALA:HB1	1:H:123:GLU:CD	2.32	0.48
1:H:13:GLU:HG2	1:H:74:VAL:HG21	1.96	0.48
1:H:245:LYS:C	1:H:247:GLN:H	2.16	0.48
1:G:342:PHE:CE1	1:G:362:THR:HG23	2.48	0.48
1:D:247:GLN:O	1:D:249:GLU:N	2.46	0.48
2:C:420:THR:HB	1:H:162:MET:HE3	1.96	0.48
1:D:68:ALA:H	1:D:91:LYS:CD	2.27	0.48
1:A:120:TYR:HB3	1:A:366:THR:HG23	1.96	0.48
1:D:158:ARG:HG3	1:E:329:ALA:CB	2.43	0.48
1:D:340:LEU:C	1:D:340:LEU:HD23	2.33	0.48
1:A:140:GLN:C	1:A:142:ASN:N	2.67	0.48
1:D:7:LYS:HB2	1:D:39:ALA:CB	2.43	0.48
1:D:36:GLU:HB3	1:D:39:ALA:HB2	1.96	0.48
1:E:156:PHE:CE2	1:E:158:ARG:HB2	2.49	0.48
1:H:3:ILE:HG23	1:H:33:VAL:HG22	1.95	0.48
1:E:135:ASP:O	1:E:137:LEU:N	2.47	0.48
1:H:147:ARG:CG	1:H:327:VAL:HG22	2.44	0.48
2:C:371:PHE:HB2	2:C:376:ILE:CG1	2.43	0.48
1:A:138:SER:OG	5:A:400:NAD:H5N	2.12	0.48
2:F:377:ASN:OD1	2:F:413:LEU:HA	2.13	0.48
1:G:354:LEU:C	1:G:354:LEU:HD23	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLY:HA2	1:B:116:LYS:O	2.14	0.48
1:H:203:VAL:HG13	5:H:400:NAD:N7A	2.28	0.48
1:D:343:LEU:O	1:D:347:VAL:HG23	2.14	0.48
1:G:97:MET:CE	1:G:343:LEU:HD13	2.43	0.48
1:E:78:MET:HA	1:E:82:GLU:OE2	2.14	0.48
1:A:180:VAL:HG12	1:A:180:VAL:O	2.14	0.48
1:B:207:THR:HA	1:B:210:GLN:HG3	1.96	0.48
1:E:37:GLN:HG2	1:E:59:SER:HA	1.95	0.48
1:H:361:GLU:HA	1:H:364:SER:OG	2.13	0.48
1:E:161:PRO:HB3	1:E:195:GLY:HA3	1.96	0.48
1:B:50:LEU:O	1:B:53:ALA:N	2.46	0.48
1:D:354:LEU:O	1:D:355:VAL:HG22	2.14	0.48
1:H:91:LYS:O	1:H:94:ALA:HB2	2.14	0.48
1:B:13:GLU:OE1	1:B:75:GLN:NE2	2.37	0.48
1:E:3:ILE:HA	1:E:70:VAL:O	2.14	0.48
1:H:98:CYS:H	1:H:122:MET:HE1	1.79	0.47
1:D:275:LEU:O	1:D:280:MET:HE1	2.14	0.47
1:D:46:THR:O	1:D:49:ALA:N	2.46	0.47
1:D:57:ILE:HD12	1:D:58:ALA:O	2.14	0.47
1:E:120:TYR:HB3	1:E:366:THR:HG22	1.96	0.47
1:A:7:LYS:H	1:A:36:GLU:CG	2.27	0.47
1:D:126:PRO:O	1:D:128:ILE:N	2.43	0.47
1:D:125:MET:CE	1:D:134:MET:HB2	2.44	0.47
1:A:21:GLU:CD	1:A:21:GLU:N	2.68	0.47
1:B:265:ALA:CB	1:B:275:LEU:HD11	2.43	0.47
1:G:332:SER:O	1:G:333:PRO:C	2.53	0.47
1:B:295:VAL:HG13	1:B:296:GLU:N	2.28	0.47
2:C:444:ASN:HD22	2:C:444:ASN:C	2.17	0.47
1:H:47:ASP:HB3	1:H:57:ILE:CG1	2.43	0.47
1:E:302:PRO:HG2	1:E:303:LEU:HD12	1.97	0.47
1:H:330:ASP:O	1:H:333:PRO:HD2	2.14	0.47
1:B:113:THR:CG2	1:B:373:ALA:HA	2.40	0.47
1:B:1:MET:HE1	1:B:353:THR:HA	1.96	0.47
2:C:425:LYS:HB3	2:C:425:LYS:HZ3	1.78	0.47
1:D:47:ASP:OD2	1:D:57:ILE:HD13	2.14	0.47
1:D:202:ASP:HB3	1:D:207:THR:HG21	1.96	0.47
1:E:123:GLU:HA	1:E:137:LEU:HD11	1.95	0.47
1:E:220:THR:O	1:E:221:VAL:C	2.52	0.47
1:D:354:LEU:C	1:D:355:VAL:CG2	2.83	0.47
1:D:322:ASN:HD22	1:D:325:SER:CB	2.16	0.47
1:A:177:VAL:O	1:A:177:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:295:GLY:HA3	2:I:446:MET:CE	2.44	0.47
1:A:158:ARG:HG3	1:B:329:ALA:HB3	1.95	0.47
1:B:325:SER:O	1:B:328:ALA:HB2	2.14	0.47
2:F:393:ASP:O	2:F:395:THR:N	2.47	0.47
1:B:72:TRP:CD2	1:B:339:LEU:HD23	2.49	0.47
1:H:128:ILE:O	1:H:132:GLN:HG2	2.14	0.47
1:H:129:SER:HA	1:H:132:GLN:NE2	2.29	0.47
2:F:405:SER:C	2:F:407:ILE:H	2.18	0.47
1:G:5:ILE:HG23	1:G:17:ALA:HB3	1.96	0.47
1:H:3:ILE:CG1	1:H:70:VAL:HG13	2.45	0.47
1:B:120:TYR:HE1	1:B:367:CYS:HB2	1.79	0.47
1:E:46:THR:O	1:E:50:LEU:HB2	2.13	0.47
1:D:199:MET:HG2	1:D:219:ILE:HD11	1.97	0.47
2:I:363:ALA:O	2:I:364:ASN:HB2	2.14	0.47
1:B:96:LEU:HD12	1:B:97:MET:N	2.29	0.47
1:E:155:GLU:HG3	1:E:318:VAL:HG21	1.96	0.47
1:G:174:ARG:HB2	1:G:258:THR:HA	1.97	0.47
1:A:5:ILE:HG21	1:A:18:ILE:HG22	1.97	0.47
1:D:130:ARG:NH1	1:D:360:ASP:OD2	2.48	0.47
1:G:346:HIS:CE1	1:G:363:VAL:CG2	2.98	0.47
1:G:248:ALA:HB1	1:G:280:MET:HE1	1.95	0.47
2:C:330:MET:HB2	2:C:460:VAL:HG22	1.97	0.47
1:E:72:TRP:HE1	1:E:97:MET:HE2	1.79	0.47
1:B:105:ASN:HB3	1:B:108:VAL:HG12	1.97	0.47
1:G:188:ILE:CG2	1:G:214:LEU:HD13	2.44	0.47
1:E:210:GLN:H	1:E:210:GLN:HG2	1.37	0.47
2:F:334:LEU:HB3	2:F:339:VAL:HB	1.96	0.47
2:I:439:LEU:C	2:I:441:PHE:N	2.68	0.47
1:D:248:ALA:HB1	1:D:280:MET:SD	2.55	0.47
1:D:221:VAL:CG2	1:D:247:GLN:HA	2.45	0.47
2:I:426:ARG:NH2	6:I:500:NDP:O3X	2.45	0.47
1:E:244:ARG:CB	1:E:244:ARG:NH2	2.75	0.47
1:D:320:HIS:CD2	1:D:326:ARG:CZ	2.98	0.47
1:H:347:VAL:O	1:H:347:VAL:HG13	2.14	0.47
1:A:207:THR:O	1:A:210:GLN:HB2	2.15	0.47
1:E:1:MET:HG2	1:E:352:LYS:O	2.13	0.47
1:B:312:LYS:HE2	1:B:313:HIS:NE2	2.30	0.47
1:A:266:LEU:O	1:A:267:ILE:HG13	2.15	0.47
1:A:1:MET:CE	1:A:1:MET:HA	2.44	0.47
2:I:397:PRO:HB3	2:I:416:GLU:OE2	2.15	0.47
1:A:28:GLY:C	1:A:30:GLY:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:416:GLU:HG3	2:C:442:ARG:HH12	1.79	0.47
1:D:68:ALA:O	1:D:91:LYS:HG2	2.14	0.47
1:H:25:LYS:HG2	1:H:340:LEU:HD21	1.97	0.47
1:A:15:ARG:NH1	1:A:324:PRO:HB2	2.30	0.47
1:E:127:ARG:HH22	1:E:132:GLN:HG3	1.78	0.47
1:B:2:LYS:N	1:B:69:ASP:OD1	2.41	0.47
1:H:112:LEU:CD1	1:H:112:LEU:H	2.28	0.47
1:A:106:ARG:O	1:A:109:VAL:N	2.47	0.47
1:G:256:VAL:HG23	1:G:257:LYS:HG3	1.97	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: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
2:I:433:ALA:O	2:I:435:VAL:N	2.47	0.47
2:I:416:GLU:OE1	2:I:442:ARG:NH1	2.48	0.47
2:F:326:ALA:O	2:F:329:GLU:HB2	2.15	0.47
1:A:377:PRO:HA	1:A:381:GLY:HA3	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:D:94:ALA:O	1:D:117:ILE:HG23	2.15	0.47
1:D:358:LEU:CD1	1:D:370:ARG:HH22	2.18	0.47
1:B:267:ILE:HG12	5:B:400:NAD:C2A	2.45	0.47
1:E:169:THR:CG2	1:E:170:VAL:N	2.77	0.47
2:C:343:TYR:N	2:C:343:TYR:CD1	2.83	0.47
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
2:F:403:PRO:HA	2:F:408:TYR:CD1	2.49	0.46
1:B:8:GLU:OE1	1:B:74:VAL:HG22	2.15	0.46
1:E:23:VAL:HG11	1:E:55:ALA:HB2	1.97	0.46
1:E:136:ILE:HD12	1:E:137:LEU:N	2.30	0.46
1:H:5:ILE:CG1	1:H:72:TRP:CD1	2.97	0.46
2:C:395:THR:OG1	2:C:415:VAL:HG21	2.15	0.46
2:C:423:PHE:C	2:C:424:ILE:HD12	2.35	0.46
1:D:351:THR:O	1:D:352:LYS:C	2.53	0.46
1:G:114:LYS:C	1:G:116:LYS:H	2.18	0.46
1: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
1:B:369:THR:HA	1:B:375:VAL:HG23	1.97	0.46
1:H:330:ASP:O	1:H:333:PRO:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:CE	2:C:357:ASN:HD21	2.29	0.46
1:G:255:LEU:HD21	1:G:276:ILE:CD1	2.45	0.46
2:C:444:ASN:ND2	2:C:444:ASN:C	2.69	0.46
2:I:396:ASN:O	2:I:412:ILE:HD13	2.15	0.46
1:B:219:ILE:O	1:B:220:THR:HG23	2.15	0.46
2:C:300:ALA:HB2	2:C:448:LEU:HD11	1.98	0.46
1:G:163:MET:HB2	1:G:170:VAL:HG13	1.94	0.46
1:D:4:ALA:CB	1:D:34:ILE:HB	2.45	0.46
1:E:25:LYS:HG2	1:E:340:LEU:HD21	1.96	0.46
1:E:136:ILE:HD11	1:E:137:LEU:HD12	1.96	0.46
1:E:178:PHE:HB2	1:E:263:THR:HA	1.96	0.46
1:D:311:VAL:O	1:D:312:LYS:HG2	2.16	0.46
1:A:23:VAL:HG22	1:A:33:VAL:HG11	1.97	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
2:C:403:PRO:HG3	2:C:408:TYR:CZ	2.51	0.46
2:F:452:ALA:H	6:F:500:NDP:C2A	2.28	0.46
1:D:280:MET:C	1:D:282:THR:N	2.69	0.46
2:C:425:LYS:CB	2:C:425:LYS:NZ	2.79	0.46
2:I:453:LYS:HE2	2:I:457:GLU:OE2	2.16	0.46
1:B:366:THR:HG22	1:B:367:CYS:N	2.30	0.46
1:E:110:GLU:O	1:E:113:THR:HB	2.15	0.46
1:E:17:ALA:O	1:E:18:ILE:HB	2.15	0.46
1:H:264:THR:O	1:H:265:ALA:C	2.53	0.46
1:H:281:VAL:HG21	1:H:303:LEU:HD11	1.98	0.46
1:H:354:LEU:H	1:H:354:LEU:CD2	2.09	0.46
1:E:341:ASN:O	1:E:345:PRO:CD	2.63	0.46
1:D:318:VAL:HG13	1:D:320:HIS:CE1	2.51	0.46
2:C:322:GLN:HE22	2:C:324:GLN:HE22	1.60	0.46
1:G:373:ALA:O	1:G:375:VAL:HG13	2.16	0.46
1:B:50:LEU:HB3	1:B:55:ALA:HB3	1.97	0.46
1:D:19:SER:OG	1:D:22:VAL:HG23	2.15	0.46
1:H:5:ILE:HD11	1:H:72:TRP:HE1	1.80	0.46
1:D:91:LYS:C	1:D:92:GLU:O	2.52	0.46
1:D:16:VAL:HG22	1:D:18:ILE:HG22	1.97	0.46
1:A:165:THR:CG2	2:C:353:PRO:HB3	2.42	0.46
2:F:328:ARG:HB3	2:F:328:ARG:CZ	2.45	0.46
1:E:344:THR:N	1:E:345:PRO:CD	2.79	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:A:351:THR:HB	1:A:353:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:VAL:HG11	1:H:319:GLY:CA	2.46	0.46
1:D:344:THR:N	1:D:345:PRO:CD	2.78	0.46
1:D:113:THR:CA	1:D:369:THR:HG21	2.46	0.46
1:H:348:ASP:N	1:H:355:VAL:HG12	2.31	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:G:47:ASP:HB3	1:G:57:ILE:HG12	1.98	0.46
1:D:146:TYR:CE2	1:E:159:ALA:HA	2.51	0.46
1:H:40:GLY:O	1:H:43:ALA:N	2.47	0.46
2:I:399:ALA:CA	2:I:408:TYR:HA	2.34	0.46
1:A:120:TYR:HD2	1:A:366:THR:HG22	1.81	0.46
1:H:218:PHE:HD2	1:H:220:THR:CG2	2.25	0.46
1:D:120:TYR:CE1	1:D:363:VAL:HG13	2.50	0.46
1:E:112:LEU:HB3	1:E:117:ILE:HB	1.98	0.46
1:H:3:ILE:HG13	1:H:70:VAL:HG13	1.97	0.46
2:C:330:MET:HG3	2:C:463:MET:CE	2.42	0.46
1:E:136:ILE:HG22	1:E:338:ASN:CB	2.45	0.46
1:D:360:ASP:C	1:D:362:THR:H	2.18	0.46
1:D:13:GLU:HA	1:D:13:GLU:OE1	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:H:210:GLN:HA	1:H:213:SER:HB3	1.97	0.46
2:F:453:LYS:HE2	2:F:457:GLU:OE2	2.16	0.46
1:E:327:VAL:HG12	1:E:327:VAL:O	2.16	0.46
1:H:7:LYS:HB2	1:H:39:ALA:HB2	1.96	0.45
1:B:346:HIS:HD1	1:B:356:MET:CE	2.29	0.45
1:E:25:LYS:CG	1:E:340:LEU:HD21	2.45	0.45
1:B:10:ARG:CG	1:B:10:ARG:HH11	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
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
2:C:416:GLU:HB3	2:C:439:LEU:HD21	1.98	0.45
1:E:162:MET:HE1	2:I:420:THR:HG23	1.99	0.45
1:A:38:GLY:N	1:A:47:ASP:OD1	2.48	0.45
1:H:192:LYS:HE2	1:H:215:GLY:HA3	1.98	0.45
1:H:131:ALA:HA	1:H:134:MET:HE3	1.97	0.45
1:H:204:ARG:C	1:H:206:ALA:H	2.20	0.45
2:I:455:MET:O	2:I:459:ILE:HG13	2.16	0.45
1:D:198:VAL:HG12	1:D:199:MET:N	2.32	0.45
1:E:130:ARG:HG2	1:E:130:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:MET:O	1:E:98:CYS:CB	2.61	0.45
1:B:295:VAL:HG11	1:B:320:HIS:O	2.16	0.45
1:H:41:VAL:HG13	1:H:42:GLY:N	2.32	0.45
1:E:147:ARG:O	1:E:148:ALA:C	2.55	0.45
2:C:366:PRO:HB2	2:C:369:GLU:HG3	1.98	0.45
1:E:368:VAL:HG12	1:E:368:VAL:O	2.16	0.45
1:D:85:ASP:OD2	1:D:88:ALA:CB	2.63	0.45
1:H:100:LEU:CB	1:H:121:ALA:HB2	2.42	0.45
1:H:181:GLY:HA2	5:H:400:NAD:H52N	1.98	0.45
1:H:208:LYS:HZ2	1:H:220:THR:CG2	2.29	0.45
2:C:330:MET:HG2	2:C:334:LEU:HD21	1.98	0.45
1:G:266:LEU:H	5:G:400:NAD:H51A	1.81	0.45
2:F:437:ASN:C	2:F:439:LEU:N	2.68	0.45
1:B:185:LEU:HD13	2:C:352:MET:HB3	1.97	0.45
1:D:255:LEU:C	1:D:257:LYS:H	2.19	0.45
1:D:29:LEU:CD2	1:D:347:VAL:HG11	2.46	0.45
2:I:437:ASN:OD1	2:I:439:LEU:HB2	2.16	0.45
2:F:318:MET:CE	2:F:324:GLN:HG2	2.47	0.45
1:H:65:LEU:O	1:H:66:SER:C	2.53	0.45
1:B:73:LYS:HB3	1:B:73:LYS:NZ	2.32	0.45
2:C:459:ILE:O	2:C:463:MET:HG3	2.16	0.45
1:G:265:ALA:HB2	1:G:275:LEU:HD11	1.99	0.45
1:E:130:ARG:HD3	2:F:409:GLY:HA3	1.99	0.45
1:A:188:ILE:HG23	1:A:198:VAL:HG11	1.98	0.45
1:D:22:VAL:HG21	1:D:336:ALA:HB1	1.97	0.45
1:B:62:ALA:C	1:B:64:ALA:H	2.19	0.45
1:H:244:ARG:NH2	1:H:275:LEU:HD21	2.32	0.45
1:D:16:VAL:HG13	1:D:16:VAL:O	2.17	0.45
1:B:354:LEU:C	1:B:354:LEU:HD23	2.36	0.45
1:E:207:THR:O	1:E:211:VAL:HG23	2.17	0.45
2:C:379:SER:O	2:C:380:PHE:C	2.54	0.45
1:G:34:ILE:HG22	1:G:64:ALA:HB1	1.97	0.45
1:A:16:VAL:HG22	1:A:18:ILE:HG22	1.97	0.45
1:D:97:MET:CE	1:D:343:LEU:HD12	2.47	0.45
2:F:401:THR:OG1	2:F:402:ASP:N	2.48	0.45
1:G:16:VAL:HG22	1:G:17:ALA:H	1.82	0.45
2:I:440:PHE:HD2	2:I:447:MET:CE	2.29	0.45
1:E:342:PHE:CD1	1:E:342:PHE:C	2.89	0.45
1:A:106:ARG:N	1:A:107:PRO:CD	2.75	0.45
1:H:62:ALA:O	1:H:66:SER:N	2.50	0.45
1:H:25:LYS:O	1:H:29:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:376:ILE:HG12	2:F:376:ILE:O	2.15	0.45
1:D:240:GLY:O	1:D:242:GLU:N	2.49	0.45
2:C:362:GLU:O	2:C:362:GLU:HG2	2.15	0.45
1:E:369:THR:CG2	1:E:369:THR:O	2.64	0.45
1:H:3:ILE:O	1:H:33:VAL:HA	2.15	0.45
1:G:221:VAL:HG12	1:G:222:ASP:H	1.80	0.45
2:I:332:ASP:O	2:I:333:VAL:C	2.54	0.45
1:B:346:HIS:O	1:B:348:ASP:N	2.49	0.45
1:B:281:VAL:HG23	1:B:313:HIS:HD2	1.81	0.45
1:G:92:GLU:HG2	1:G:92:GLU:H	1.52	0.45
1:H:245:LYS:C	1:H:247:GLN:N	2.70	0.45
1:D:164:MET:HE2	1:D:169:THR:HG23	1.99	0.45
2:F:300:ALA:O	2:F:304:MET:HE2	2.17	0.45
1:D:252:LEU:HD11	1:D:283:LYS:HD3	1.99	0.45
1:E:267:ILE:HG12	1:E:273:PRO:HD3	1.98	0.45
2:C:418:ALA:O	2:C:419:GLY:C	2.55	0.45
1:B:79:THR:O	1:B:84:THR:O	2.35	0.45
1:D:23:VAL:O	1:D:26:LEU:HB2	2.17	0.45
1:D:332:SER:CB	1:D:333:PRO:HD3	2.45	0.45
2:F:445:THR:CG2	2:F:446:MET:N	2.80	0.45
1: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:G:63:GLN:OE1	1:G:63:GLN:HA	2.16	0.45
1:B:87:VAL:C	1:B:89:LEU:H	2.20	0.45
1:D:160:PHE:CZ	1:D:260:ILE:HD12	2.51	0.45
1:H:63:GLN:CA	1:H:63:GLN:HE21	2.21	0.45
2:C:309:LYS:HE2	2:C:382:THR:O	2.17	0.45
2:I:299:ASP:O	2:I:303:ILE:HG13	2.17	0.45
1:A:3:ILE:HG13	1:A:70:VAL:HG13	1.99	0.45
1:G:270:LYS:N	1:G:270:LYS:HD2	2.31	0.45
1:B:276:ILE:O	1:B:301:CYS:HA	2.17	0.45
1:H:120:TYR:CB	1:H:366:THR:HG23	2.47	0.44
1:H:99:HIS:CE1	1:H:123:GLU:HB3	2.52	0.44
1:H:356:MET:O	1:H:358:LEU:N	2.50	0.44
1:D:3:ILE:HB	1:D:70:VAL:CG2	2.47	0.44
1:H:66:SER:HB3	1:H:67:GLN:NE2	2.32	0.44
1:D:57:ILE:HD12	1:D:58:ALA:N	2.30	0.44
1:G:101:GLY:N	1:G:123:GLU:OE2	2.50	0.44
1:B:105:ASN:O	1:B:108:VAL:HG12	2.17	0.44
2:C:385:VAL:HG12	2:C:386:ALA:N	2.32	0.44
1:D:65:LEU:HD22	1:D:71:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:325:SER:C	1:H:327:VAL:H	2.20	0.44
1:E:272:ALA:HB3	1:E:299:GLY:H	1.82	0.44
1:H:125:MET:HG3	1:H:131:ALA:HB1	1.97	0.44
1:G:121:ALA:HB1	1:G:123:GLU:OE1	2.16	0.44
2:C:420:THR:HG21	1:H:169:THR:OG1	2.18	0.44
1:B:244:ARG:HD3	1:B:244:ARG:N	2.28	0.44
1:E:284:MET:HE3	1:E:315:VAL:HG21	1.99	0.44
1:E:143:LEU:HD13	1:E:327:VAL:HG11	2.00	0.44
1:A:18:ILE:N	1:A:336:ALA:HB2	2.32	0.44
1:H:113:THR:HG21	1:H:374:ILE:CG1	2.43	0.44
1:D:362:THR:O	1:D:362:THR:CG2	2.65	0.44
1:D:277:THR:O	1:D:280:MET:N	2.46	0.44
1:A:167:ALA:HB2	1:B:338:ASN:ND2	2.31	0.44
1:D:205:ALA:C	1:D:207:THR:N	2.71	0.44
1:B:147:ARG:HH11	1:B:151:ASP:CG	2.19	0.44
1:E:132:GLN:O	1:E:133:SER:C	2.56	0.44
2:I:396:ASN:HA	2:I:397:PRO:HD2	1.85	0.44
1:E:273:PRO:O	1:E:274:VAL:C	2.55	0.44
1:H:72:TRP:CA	1:H:97:MET:O	2.64	0.44
1:A:277:THR:C	1:A:279:GLU:H	2.20	0.44
1:A:161:PRO:CB	1:B:193:ARG:HH12	2.29	0.44
1:G:200:ALA:HB3	1:G:211:VAL:CG1	2.47	0.44
1:D:43:ALA:O	1:D:44:SER:HB2	2.18	0.44
2:F:442:ARG:HH11	2:F:442:ARG:HG3	1.82	0.44
1:D:149:VAL:HG11	1:D:190:THR:HG22	1.99	0.44
1:B:3:ILE:O	1:B:3:ILE:HG23	2.17	0.44
1:H:75:GLN:O	1:H:76:ARG:C	2.55	0.44
2:C:401:THR:O	2:C:408:TYR:CE2	2.71	0.44
2:C:373:LEU:HD11	2:C:411:PRO:HB2	1.99	0.44
1:G:121:ALA:HB3	1:G:124:LEU:CD1	2.45	0.44
2:F:347:PRO:HD3	2:F:373:LEU:HB2	1.98	0.44
1:E:7:LYS:HE3	1:E:8:GLU:O	2.18	0.44
1:E:160:PHE:CE1	1:E:260:ILE:HD12	2.52	0.44
2:F:305:LYS:NZ	2:F:337:GLU:HG3	2.33	0.44
1:D:294:ALA:O	1:D:299:GLY:HA2	2.17	0.44
2:C:373:LEU:HG	2:C:377:ASN:HD21	1.81	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:E:338:ASN:HD22	1:E:338:ASN:HA	1.64	0.44
1:A:161:PRO:HB3	1:B:193:ARG:NH1	2.32	0.44
1:D:9:ARG:CB	1:D:9:ARG:HH11	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LEU:HD22	1:E:167:ALA:HB1	1.99	0.44
1:H:119:ALA:H	1:H:369:THR:HG23	1.83	0.44
1:H:122:MET:SD	1:H:122:MET:N	2.91	0.44
1:D:362:THR:O	1:D:362:THR:HG23	2.17	0.44
1:G:16:VAL:HG22	1:G:17:ALA:N	2.33	0.44
1:G:10:ARG:CG	1:G:75:GLN:HG2	2.46	0.44
1:A:105:ASN:C	1:A:107:PRO:HD2	2.38	0.44
1:A:176:LEU:HD13	1:A:178:PHE:CZ	2.53	0.44
1:G:247:GLN:C	1:G:249:GLU:H	2.21	0.44
1:G:278:GLU:HG3	1:G:303:LEU:CD1	2.48	0.44
1:G:165:THR:CG2	2:I:353:PRO:HB3	2.47	0.44
1:E:122:MET:HE2	1:E:339:LEU:HG	1.99	0.44
1:A:118:THR:HA	1:A:369:THR:O	2.18	0.44
1:A:359:GLU:H	1:A:359:GLU:CD	2.21	0.44
1:H:284:MET:CE	1:H:290:ILE:HD11	2.48	0.44
1:H:33:VAL:HB	1:H:55:ALA:HB2	1.99	0.44
1:B:71:VAL:CG1	1:B:96:LEU:HD13	2.48	0.44
1:G:184:GLY:O	1:G:188:ILE:HG13	2.17	0.44
1:E:51:THR:CG2	1:E:57:ILE:HG23	2.48	0.44
1:A:337:LYS:HZ2	1:B:168:GLY:HA3	1.82	0.44
2:C:292:HIS:O	2:C:292:HIS:CD2	2.71	0.44
1:H:19:SER:HB3	1:H:22:VAL:HB	2.00	0.44
1:H:10:ARG:HH22	1:H:82:GLU:CD	2.21	0.44
1:D:203:VAL:O	1:D:228:THR:HB	2.17	0.44
1:B:121:ALA:HB3	1:B:124:LEU:HD12	1.98	0.44
1:G:37:GLN:HE21	1:G:59:SER:HA	1.82	0.44
2:C:438:GLU:O	2:C:438:GLU:HG2	2.17	0.44
1:A:354:LEU:HD21	1:A:356:MET:HE1	1.93	0.43
1:A:175:VAL:HG12	1:A:176:LEU:N	2.33	0.43
1:D:24:LYS:C	1:D:26:LEU:H	2.21	0.43
1:B:100:LEU:O	1:B:101:GLY:C	2.56	0.43
1:D:109:VAL:CG2	1:D:110:GLU:N	2.81	0.43
1:G:110:GLU:O	1:G:114:LYS:HG2	2.18	0.43
1:A:351:THR:O	1:A:352:LYS:C	2.56	0.43
1:H:368:VAL:HG22	1:H:376:HIS:HB2	2.00	0.43
1:A:120:TYR:CZ	1:A:356:MET:HG2	2.53	0.43
1:H:346:HIS:HB3	1:H:356:MET:HA	1.99	0.43
1:G:10:ARG:HG3	1:G:11:PRO:HD2	2.00	0.43
1:E:117:ILE:O	1:E:369:THR:HG23	2.18	0.43
1:H:67:GLN:N	1:H:67:GLN:NE2	2.56	0.43
1:E:100:LEU:HD12	1:E:121:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:VAL:CA	1:H:355:VAL:HG12	2.47	0.43
1:A:139:SER:OG	1:A:338:ASN:ND2	2.42	0.43
1:G:208:LYS:HZ2	1:G:218:PHE:HD2	1.66	0.43
1:E:7:LYS:HB2	1:E:39:ALA:CA	2.48	0.43
1:G:214:LEU:HA	1:G:214:LEU:HD23	1.85	0.43
1:B:129:SER:O	1:B:132:GLN:HG3	2.17	0.43
1:G:329:ALA:HB3	1:H:157:ALA:O	2.18	0.43
1:D:2:LYS:HZ3	1:D:32:GLU:HG2	1.83	0.43
2:C:330:MET:HB2	2:C:460:VAL:CG2	2.48	0.43
1:E:346:HIS:HB3	1:E:356:MET:HA	1.99	0.43
1:D:194:LEU:CD2	1:E:194:LEU:HD13	2.47	0.43
1:G:200:ALA:O	1:G:218:PHE:HA	2.19	0.43
1:G:156:PHE:CZ	1:G:259:ASP:HB3	2.54	0.43
2:F:298:GLU:H	2:F:298:GLU:CD	2.22	0.43
1:E:247:GLN:O	1:E:251:VAL:HG23	2.18	0.43
1:D:241:GLU:O	1:D:241:GLU:OE2	2.36	0.43
1:H:120:TYR:CB	1:H:366:THR:HG21	2.45	0.43
2:C:326:ALA:HB1	2:C:456:THR:HB	2.01	0.43
1:G:199:MET:HE3	1:G:217:LYS:HB2	2.00	0.43
1:D:348:ASP:OD2	1:D:353:THR:N	2.46	0.43
1:G:244:ARG:O	1:G:244:ARG:CG	2.65	0.43
1:A:357:LYS:O	1:A:359:GLU:OE2	2.36	0.43
2:C:405:SER:HA	2:C:406:PRO:HD3	1.73	0.43
1:B:62:ALA:C	1:B:64:ALA:N	2.72	0.43
1:H:128:ILE:HD11	1:H:131:ALA:H	1.84	0.43
1:H:73:LYS:CD	1:H:75:GLN:O	2.66	0.43
1:E:23:VAL:CG1	1:E:55:ALA:HB2	2.49	0.43
1:H:213:SER:OG	2:I:355:HIS:CE1	2.71	0.43
1:D:100:LEU:O	1:D:102:ALA:N	2.51	0.43
1:B:36:GLU:O	1:B:39:ALA:HB2	2.18	0.43
1:D:9:ARG:NH1	1:D:9:ARG:HB3	2.33	0.43
1:E:220:THR:HG23	1:E:221:VAL:N	2.34	0.43
1:D:255:LEU:C	1:D:257:LYS:N	2.71	0.43
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.82	0.43
1:H:18:ILE:HG12	1:H:19:SER:H	1.83	0.43
1:B:85:ASP:OD1	1:B:88:ALA:CB	2.66	0.43
1:H:66:SER:CB	1:H:67:GLN:NE2	2.81	0.43
1:D:5:ILE:HD13	1:D:18:ILE:HG13	2.01	0.43
1:G:26:LEU:O	1:G:29:LEU:HB2	2.18	0.43
1:D:264:THR:CG2	1:D:293:LEU:HD12	2.44	0.43
1:B:99:HIS:CD2	1:B:99:HIS:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:THR:O	1:G:208:LYS:C	2.57	0.43
1:E:370:ARG:O	1:E:371:ASP:C	2.57	0.43
1:D:193:ARG:C	1:D:195:GLY:H	2.22	0.43
1:E:280:MET:O	1:E:283:LYS:N	2.45	0.43
1:E:190:THR:O	1:E:191:ALA:C	2.56	0.43
1:A:62:ALA:HA	1:A:89:LEU:HD22	2.00	0.43
2:C:377:ASN:OD1	2:C:413:LEU:HA	2.19	0.43
1:D:175:VAL:HG23	1:D:196:ALA:HB1	2.01	0.43
1:B:134:MET:HE1	1:B:362:THR:HG21	2.00	0.43
2:F:416:GLU:HG3	2:F:439:LEU:CD1	2.48	0.43
1:B:2:LYS:HE3	1:B:32:GLU:OE1	2.18	0.43
1:H:113:THR:C	1:H:115:ARG:H	2.20	0.43
1:H:128:ILE:HD11	1:H:131:ALA:CB	2.48	0.43
1:H:185:LEU:O	1:H:214:LEU:CD1	2.67	0.43
1:H:282:THR:HG22	1:H:313:HIS:NE2	2.34	0.43
1:H:346:HIS:CB	1:H:356:MET:HA	2.48	0.43
1:D:356:MET:HB3	1:D:363:VAL:HG11	2.00	0.43
1:G:247:GLN:O	1:G:249:GLU:N	2.52	0.43
1:H:29:LEU:HD21	1:H:344:THR:HG22	2.01	0.43
1:A:205:ALA:C	1:A:207:THR:N	2.72	0.43
1:D:211:VAL:HG12	1:D:216:GLY:O	2.19	0.43
1: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:D:361:GLU:CA	1:D:364:SER:HB3	2.31	0.43
2:F:352:MET:N	6:F:500:NDP:N7N	2.66	0.43
1:D:292:ASP:OD2	1:D:300:ASN:N	2.52	0.43
1:D:175:VAL:HA	1:D:260:ILE:O	2.19	0.43
1:A:291:ILE:CD1	1:A:318:VAL:HB	2.40	0.43
1:D:147:ARG:HG2	1:D:323:VAL:HG13	2.01	0.43
1:E:120:TYR:HA	1:E:367:CYS:HA	2.00	0.43
1:B:308:LYS:CG	1:B:309:ILE:H	2.26	0.43
1:D:78:MET:CE	1:D:82:GLU:HG2	2.49	0.43
1:B:202:ASP:OD1	1:B:203:VAL:N	2.51	0.43
2:F:437:ASN:O	2:F:439:LEU:N	2.52	0.43
1:B:152:GLY:HA2	1:B:291:ILE:HD11	2.01	0.43
2:F:316:TYR:HB2	2:F:350:GLY:HA2	2.00	0.43
1:B:357:LYS:O	1:B:360:ASP:HB3	2.19	0.43
2:F:460:VAL:HG12	2:F:460:VAL:O	2.19	0.43
1:G:95:VAL:HA	1:G:118:THR:O	2.18	0.43
1:H:355:VAL:CG1	1:H:355:VAL:O	2.65	0.43
1:B:210:GLN:HE22	2:C:351:ARG:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:LYS:HA	1:H:286:PRO:HD3	1.80	0.43
1:B:87:VAL:HG13	1:B:88:ALA:H	1.81	0.42
1:B:130:ARG:HG3	1:B:130:ARG:H	1.44	0.42
1:H:65:LEU:HB3	1:H:90:ILE:HA	2.01	0.42
1:E:4:ALA:HA	1:E:34:ILE:O	2.19	0.42
1:A:343:LEU:HD23	1:A:343:LEU:C	2.39	0.42
2:F:430:SER:OG	2:F:434:GLY:HA2	2.19	0.42
1:A:245:LYS:HA	1:A:245:LYS:HD2	1.86	0.42
1:A:78:MET:HG3	1:A:86:GLU:OE1	2.19	0.42
1:D:121:ALA:HB1	1:D:124:LEU:HD22	2.01	0.42
1:G:380:THR:CG2	1:G:380:THR:O	2.68	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:H:323:VAL:N	1:H:324:PRO:CD	2.82	0.42
1:H:148:ALA:HB1	1:H:262:ILE:HG21	2.00	0.42
1:B:88:ALA:HA	1:B:115:ARG:HD2	2.01	0.42
1:H:72:TRP:CB	1:H:97:MET:HB2	2.25	0.42
1:D:68:ALA:N	1:D:91:LYS:CD	2.83	0.42
1:D:163:MET:HE2	1:D:163:MET:HB2	1.84	0.42
1:G:97:MET:O	1:G:98:CYS:HB3	2.18	0.42
1:E:97:MET:HE2	1:E:343:LEU:HD12	2.00	0.42
1:A:136:ILE:HA	1:A:338:ASN:ND2	2.34	0.42
1:E:309:ILE:HG23	1:E:318:VAL:HG22	2.00	0.42
2:F:292:HIS:O	2:F:293:MET:CB	2.68	0.42
1:D:127:ARG:NE	1:D:235:TYR:CE2	2.87	0.42
1:D:26:LEU:HD23	1:D:26:LEU:HA	1.89	0.42
1:D:18:ILE:CD1	1:D:50:LEU:HD23	2.50	0.42
1:E:23:VAL:HG21	1:E:50:LEU:CD1	2.49	0.42
1:H:71:VAL:O	1:H:96:LEU:HA	2.20	0.42
1:A: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:343:LEU:HD23	1:D:347:VAL:HG22	2.02	0.42
1:D:263:THR:HB	1:D:300:ASN:HB2	2.02	0.42
1:E:112:LEU:HD12	1:E:112:LEU:N	2.32	0.42
1:G:243:PHE:C	1:G:245:LYS:N	2.64	0.42
1:G:172:PRO:HB3	2:I:367:TYR:HE2	1.84	0.42
1:B:348:ASP:CG	1:B:351:THR:HB	2.40	0.42
1:G:118:THR:HB	1:G:370:ARG:HA	2.02	0.42
1:E:362:THR:CG2	1:E:363:VAL:HG23	2.50	0.42
1:A:118:THR:HA	1:A:370:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:380:PHE:O	2:I:383:ALA:HB3	2.20	0.42
2:F:296:SER:OG	2:F:298:GLU:HG2	2.20	0.42
1:D:231:THR:O	1:D:232:ALA:C	2.58	0.42
1:A:73:LYS:HB3	1:A:73:LYS:HE3	1.76	0.42
1:B:78:MET:N	1:B:86:GLU:OE1	2.47	0.42
1:D:120:TYR:CZ	1:D:356:MET:HG2	2.54	0.42
2:I:454:LYS:HG3	2:I:455:MET:N	2.35	0.42
1:E:106:ARG:N	1:E:107:PRO:CD	2.82	0.42
1:E:268:PRO:O	1:E:270:LYS:N	2.53	0.42
1:A:5:ILE:O	1:A:35:VAL:HA	2.19	0.42
1:B:197:VAL:HG12	1:B:197:VAL:O	2.19	0.42
1:B:303:LEU:HB2	1:B:317:ILE:HD13	2.01	0.42
1:G:76:ARG:HD3	1:G:100:LEU:O	2.19	0.42
1:D:247:GLN:C	1:D:249:GLU:H	2.23	0.42
1:E:121:ALA:C	1:E:366:THR:HG23	2.40	0.42
1:G:295:VAL:HG21	1:G:306:PRO:HA	2.01	0.42
1:H:370:ARG:O	1:H:371:ASP:C	2.57	0.42
1:A:362:THR:HG22	1:A:363:VAL:HG23	2.01	0.42
1:G:128:ILE:C	1:G:130:ARG:H	2.23	0.42
1:A:177:VAL:HA	1:A:262:ILE:O	2.19	0.42
1:D:72:TRP:CE2	1:D:339:LEU:HB3	2.54	0.42
2:I:393:ASP:OD2	6:I:500:NDP:O3D	2.35	0.42
1:A:327:VAL:O	1:A:328:ALA:C	2.58	0.42
1:D:204:ARG:O	1:D:206:ALA:N	2.53	0.42
1:D:320:HIS:CD2	1:D:326:ARG:NH2	2.88	0.42
1:B:281:VAL:HG23	1:B:313:HIS:CD2	2.54	0.42
1:A:290:ILE:HD12	1:A:317:ILE:CD1	2.49	0.42
2:I:405:SER:OG	2:I:406:PRO:HD2	2.20	0.42
1:H:22:VAL:HG21	1:H:336:ALA:HB1	2.02	0.42
1:B:58:ALA:HB3	1:B:64:ALA:HB2	2.01	0.42
1:H:281:VAL:CG2	1:H:282:THR:N	2.83	0.42
2:C:399:ALA:HB2	2:C:407:ILE:CD1	2.49	0.42
1:D:51:THR:OG1	1:D:57:ILE:HG22	2.20	0.42
1:A:302:PRO:HG2	1:A:303:LEU:HD12	2.02	0.42
2:I:318:MET:O	2:I:322:GLN:N	2.52	0.42
1:E:138:SER:O	1:E:139:SER:C	2.58	0.42
1:B:187:ALA:O	1:B:188:ILE:C	2.57	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:B:80:ALA:HB2	1:B:85:ASP:OD2	2.20	0.42
1:D:356:MET:SD	1:D:356:MET:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:429:ALA:HB3	6:F:500:NDP:O1X	2.18	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
2:C:394:VAL:HG22	6:C:500:NDP:O1N	2.20	0.42
2:C:415:VAL:C	2:C:417:LYS:H	2.23	0.42
2:F:439:LEU:C	2:F:441:PHE:H	2.24	0.42
1:B:67:GLN:OE1	1:B:67:GLN:N	2.44	0.42
1:E:143:LEU:HD13	1:E:327:VAL:CG1	2.50	0.42
1:E:325:SER:C	1:E:327:VAL:H	2.23	0.42
1:A:3:ILE:HD13	1:A:26:LEU:HD13	2.02	0.42
1:H:46:THR:OG1	1:H:49:ALA:CB	2.68	0.42
1:D:17:ALA:O	1:D:18:ILE:HB	2.19	0.41
1:H:340:LEU:CD1	1:H:344:THR:CG2	2.98	0.41
1:A:368:VAL:O	1:A:368:VAL:HG12	2.20	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:A:179:GLY:O	1:A:184:GLY:HA3	2.20	0.41
2:C:416:GLU:HB3	2:C:439:LEU:CD2	2.50	0.41
1:B:352:LYS:HG2	1:B:352:LYS:O	2.20	0.41
1:B:58:ALA:CB	1:B:64:ALA:HA	2.51	0.41
1:A:342:PHE:CD2	1:A:342:PHE:C	2.93	0.41
1:H:208:LYS:O	1:H:212:GLU:HB2	2.20	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:D:294:ALA:C	1:D:299:GLY:HA2	2.40	0.41
1:E:95:VAL:CG1	1:E:118:THR:HB	2.39	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
2:C:426:ARG:O	2:C:449:PHE:HD1	2.02	0.41
1:H:362:THR:HG23	1:H:363:VAL:HG23	2.02	0.41
1:D:356:MET:HB3	1:D:363:VAL:HG21	2.02	0.41
1:A:330:ASP:O	1:A:333:PRO:HD2	2.19	0.41
2:F:365:VAL:O	2:F:366:PRO:C	2.59	0.41
1:E:3:ILE:CG2	1:E:33:VAL:HG22	2.50	0.41
1:H:143:LEU:HA	1:H:143:LEU:HD23	1.81	0.41
1:G:20:PRO:HD3	1:G:45:ILE:HD13	2.03	0.41
1:D:156:PHE:CZ	1:D:259:ASP:HB3	2.55	0.41
1:H:241:GLU:CG	1:H:244:ARG:HB2	2.49	0.41
1:B:106:ARG:HH12	1:B:374:ILE:CD1	2.34	0.41
1:G:153:ALA:HA	1:G:160:PHE:HE1	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:ALA:HA	5:G:400:NAD:O4B	2.19	0.41
1:A:118:THR:HG23	1:A:370:ARG:HB3	2.03	0.41
1:E:16:VAL:O	1:E:16:VAL:HG13	2.20	0.41
1:B:36:GLU:O	1:B:37:GLN:C	2.58	0.41
1:G:176:LEU:HD13	1:G:178:PHE:HE2	1.86	0.41
1:G:361:GLU:H	1:G:361:GLU:HG2	1.48	0.41
2:I:402:ASP:OD1	2:I:405:SER:HB2	2.19	0.41
1:H:368:VAL:HG12	1:H:374:ILE:HG23	2.03	0.41
1:H:73:LYS:HG3	1:H:98:CYS:SG	2.61	0.41
1:G:346:HIS:ND1	1:G:356:MET:CE	2.84	0.41
1:G:9:ARG:O	1:G:10:ARG:C	2.59	0.41
1:H:29:LEU:N	1:H:29:LEU:HD12	2.35	0.41
1:D:224:GLU:N	1:D:227:LYS:HG2	2.35	0.41
1:D:164:MET:CE	1:D:169:THR:HG23	2.50	0.41
1:B:181:GLY:O	1:B:182:VAL:C	2.59	0.41
1:D:100:LEU:C	1:D:102:ALA:N	2.74	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:H:249:GLU:C	1:H:251:VAL:H	2.23	0.41
1:D:204:ARG:C	1:D:206:ALA:N	2.73	0.41
1:D:222:ASP:O	1:D:227:LYS:HE3	2.21	0.41
1:H:348:ASP:HB3	1:H:353:THR:HG22	2.02	0.41
1:A:205:ALA:C	1:A:207:THR:H	2.24	0.41
1:E:348:ASP:OD1	1:E:352:LYS:N	2.53	0.41
1:E:289:VAL:HA	1:E:316:LYS:O	2.20	0.41
1:E:212:GLU:C	1:E:214:LEU:H	2.23	0.41
1:G:122:MET:HG3	1:G:339:LEU:HD21	2.02	0.41
1:E:330:ASP:O	1:E:333:PRO:HD2	2.20	0.41
2:I:407:ILE:O	2:I:409:GLY:N	2.53	0.41
1:H:180:VAL:HB	1:H:202:ASP:OD2	2.20	0.41
1:D:122:MET:C	1:D:124:LEU:N	2.74	0.41
1:G:346:HIS:HE1	1:G:363:VAL:CG2	2.34	0.41
1:B:73:LYS:HZ2	1:B:73:LYS:CB	2.33	0.41
1:B:10:ARG:HH12	1:B:76:ARG:HG2	1.85	0.41
2:F:454:LYS:CG	2:F:455:MET:N	2.83	0.41
1:A:138:SER:OG	5:A:400:NAD:C5N	2.68	0.41
1:B:299:GLY:C	1:B:301:CYS:H	2.23	0.41
2:C:331:ALA:O	2:C:335:LYS:HG3	2.20	0.41
1:G:3:ILE:HG13	1:G:70:VAL:HG13	2.03	0.41
1:E:353:THR:HG22	1:E:354:LEU:O	2.20	0.41
1:H:277:THR:O	1:H:278:GLU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG12	1:B:131:ALA:HB2	2.02	0.41
2:C:424:ILE:CD1	2:C:424:ILE:N	2.82	0.41
1:E:358:LEU:CD1	1:E:358:LEU:H	2.15	0.41
1:D:244:ARG:H	1:D:244:ARG:HD3	1.85	0.41
1:G:249:GLU:HA	1:G:249:GLU:OE1	2.21	0.41
1:G:280:MET:C	1:G:282:THR:N	2.72	0.41
1:H:25:LYS:CA	1:H:25:LYS:HE3	2.51	0.41
1:B:134:MET:HG2	1:B:342:PHE:CA	2.51	0.41
1:B:208:LYS:NZ	1:B:212:GLU:OE2	2.45	0.41
1:E:343:LEU:HD23	1:E:343:LEU:C	2.41	0.41
1:E:284:MET:HE1	1:E:290:ILE:HD11	2.02	0.41
1:G:96:LEU:HB3	1:G:119:ALA:CB	2.51	0.41
1:A:158:ARG:HG2	1:A:158:ARG:HH11	1.85	0.41
1:D:349:LYS:N	1:D:349:LYS:HD2	2.35	0.41
1:D:62:ALA:O	1:D:66:SER:HB3	2.20	0.41
1:H:50:LEU:HD12	1:H:50:LEU:HA	1.93	0.41
2:F:425:LYS:HB2	6:F:500:NDP:O2X	2.21	0.41
2:C:414:ASP:HB3	2:C:417:LYS:HG3	2.02	0.41
1:D:175:VAL:CG1	1:D:176:LEU:H	2.24	0.41
1:G:277:THR:C	1:G:279:GLU:N	2.74	0.41
1:D:35:VAL:HG21	1:D:50:LEU:CD2	2.49	0.41
1:H:15:ARG:CG	1:H:15:ARG:NH2	2.83	0.41
2:I:425:LYS:HE2	2:I:425:LYS:HB3	1.75	0.41
1:D:65:LEU:HD23	1:D:65:LEU:N	2.36	0.41
1:G:176:LEU:HG	1:G:199:MET:HB3	2.03	0.41
1:E:7:LYS:HB2	1:E:39:ALA:HB2	2.01	0.41
1:A:340:LEU:HA	1:A:340:LEU:HD12	1.77	0.41
1:E:103:LEU:O	1:E:104:THR:HG23	2.20	0.41
1:H:317:ILE:N	1:H:317:ILE:HD12	2.36	0.41
1:E:311:VAL:HG13	1:E:311:VAL:O	2.20	0.41
1:D:138:SER:HA	1:D:141:SER:HB3	2.03	0.41
2:C:328:ARG:C	2:C:328:ARG:HD2	2.40	0.41
2:C:399:ALA:CB	2:C:407:ILE:HG13	2.33	0.41
1:G:128:ILE:HG13	1:G:130:ARG:H	1.86	0.41
1:A:178:PHE:HB2	1:A:263:THR:HG22	2.01	0.41
1:H:2:LYS:O	1:H:70:VAL:HG12	2.21	0.41
1:H:61:ALA:O	1:H:65:LEU:HD13	2.20	0.41
1:D:223:ASP:HB2	1:D:228:THR:OG1	2.21	0.41
1:D:15:ARG:NH1	1:D:324:PRO:HB2	2.36	0.41
1:E:110:GLU:O	1:E:114:LYS:HG3	2.20	0.41
1:A:45:ILE:HG22	1:A:50:LEU:CD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ARG:O	1:D:195:GLY:N	2.54	0.41
1:D:305:GLU:HA	1:D:306:PRO:HD2	1.89	0.41
1:A:158:ARG:HB3	1:B:330:ASP:OD2	2.21	0.41
1:H:143:LEU:HD12	1:H:331:ALA:HA	2.03	0.41
1:B:155:GLU:HA	3:B:600:SUC:H6'1	2.02	0.41
2:F:321:ALA:O	2:F:322:GLN:HB2	2.21	0.41
1:E:213:SER:O	2:F:322:GLN:NE2	2.54	0.41
1:E:84:THR:O	1:E:84:THR:HG23	2.20	0.41
1:B:5:ILE:CG2	1:B:17:ALA:HB3	2.51	0.40
1:A:362:THR:CG2	1:A:363:VAL:N	2.83	0.40
1:H:346:HIS:NE2	1:H:362:THR:CG2	2.83	0.40
1:E:87:VAL:HG22	1:E:87:VAL:O	2.20	0.40
2:C:425:LYS:NZ	6:C:500:NDP:O2B	2.54	0.40
1:H:91:LYS:HB2	1:H:91:LYS:HE3	1.87	0.40
2:C:454:LYS:CE	2:C:454:LYS:HA	2.43	0.40
1:E:72:TRP:CZ2	1:E:339:LEU:HB3	2.56	0.40
1:B:267:ILE:HG12	5:B:400:NAD:N1A	2.36	0.40
1:D:125:MET:SD	1:D:126:PRO:HD2	2.61	0.40
1:H:178:PHE:HD1	1:H:263:THR:HG22	1.87	0.40
1:G:308:LYS:HD3	1:G:308:LYS:N	2.36	0.40
1:B:158:ARG:HE	1:B:158:ARG:HB3	1.70	0.40
1:B:24:LYS:HG3	1:B:24:LYS:H	1.68	0.40
1:B:336:ALA:O	1:B:339:LEU:HB2	2.20	0.40
2:F:432:TYR:CD2	6:F:500:NDP:H6N	2.55	0.40
1:A:309:ILE:HG13	1:A:318:VAL:HG13	2.03	0.40
1:H:51:THR:C	1:H:53:ALA:H	2.25	0.40
2:I:301:ALA:O	2:I:305:LYS:HG2	2.21	0.40
2:F:345:ILE:CG1	2:F:370:VAL:HG13	2.51	0.40
2:I:318:MET:HB2	2:I:323:ALA:HB3	2.03	0.40
1:H:267:ILE:HA	1:H:268:PRO:HD2	1.86	0.40
1:D:71:VAL:HB	1:D:96:LEU:HD12	2.03	0.40
1:B:267:ILE:HD13	5:B:400:NAD:N1A	2.37	0.40
1:B:282:THR:HG22	1:B:313:HIS:CG	2.56	0.40
1:D:100:LEU:O	1:D:101:GLY:C	2.60	0.40
1:A:208:LYS:O	1:A:212:GLU:HG3	2.21	0.40
1:G:47:ASP:O	1:G:51:THR:HG23	2.21	0.40
1:A:122:MET:C	1:A:124:LEU:H	2.24	0.40
1:A:28:GLY:C	1:A:30:GLY:N	2.74	0.40
1:B:2:LYS:HB2	1:B:69:ASP:OD1	2.21	0.40
1:B:360:ASP:OD2	1:B:360:ASP:C	2.58	0.40
1:G:159:ALA:HA	1:H:146:TYR:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:443:ASN:ND2	1:H:196:ALA:O	2.54	0.40
1:H:349:LYS:HG2	1:H:349:LYS:H	1.58	0.40
1:H:26:LEU:HD21	1:H:72:TRP:HZ2	1.85	0.40
1:E:96:LEU:HD22	1:E:112:LEU:CD2	2.51	0.40
1:A:368:VAL:O	1:A:374:ILE:HG23	2.22	0.40
1:B:147:ARG:HD3	1:B:151:ASP:OD2	2.20	0.40
2:I:318:MET:HE1	2:I:324:GLN:HB3	2.04	0.40
5:B:400:NAD:O3B	5:B:400:NAD:O1N	2.25	0.40
1:A:204:ARG:O	1:A:207:THR:HB	2.22	0.40
1:H:147:ARG:HG3	1:H:327:VAL:CG2	2.50	0.40
1:A:22:VAL:O	1:A:25:LYS:N	2.55	0.40
1:B:327:VAL:O	1:B:329:ALA:N	2.55	0.40
1:A:18:ILE:HD11	1:A:23:VAL:HG23	2.04	0.40
1:G:136:ILE:HG13	1:G:137:LEU:N	2.36	0.40
1:H:203:VAL:HG22	5:H:400:NAD:C8A	2.51	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:G:69:ASP:O	1:G:94:ALA:HB1	2.22	0.40
2:C:309:LYS:HE3	2:C:383:ALA:HB2	2.02	0.40
1:E:143:LEU:CD1	1:E:331:ALA:HB2	2.51	0.40
1:G:7:LYS:CG	1:G:39:ALA:HA	2.51	0.40
1:G:99:HIS:HB2	1:G:136:ILE:CD1	2.51	0.40
1:H:270:LYS:HB2	1:H:271:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/384 (94%)	289 (80%)	51 (14%)	19 (5%)	2	14
1	B	355/384 (92%)	273 (77%)	57 (16%)	25 (7%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	376/384 (98%)	277 (74%)	66 (18%)	33 (9%)	1	5
1	E	355/384 (92%)	265 (75%)	66 (19%)	24 (7%)	1	8
1	G	360/384 (94%)	292 (81%)	50 (14%)	18 (5%)	3	16
1	H	353/384 (92%)	258 (73%)	77 (22%)	18 (5%)	2	15
2	C	172/174 (99%)	133 (77%)	35 (20%)	4 (2%)	8	35
2	F	171/174 (98%)	141 (82%)	21 (12%)	9 (5%)	2	14
2	I	171/174 (98%)	125 (73%)	29 (17%)	17 (10%)	1	4
All	All	2672/2826 (95%)	2053 (77%)	452 (17%)	167 (6%)	2	10

All (167) Ramachandran outliers are listed below:

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

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

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/296 (96%)	254 (89%)	30 (11%)	8	31
1	B	281/296 (95%)	253 (90%)	28 (10%)	9	34
1	D	293/296 (99%)	255 (87%)	38 (13%)	5	21
1	E	281/296 (95%)	257 (92%)	24 (8%)	13	45
1	G	284/296 (96%)	260 (92%)	24 (8%)	13	45
1	H	280/296 (95%)	243 (87%)	37 (13%)	5	20
2	C	138/138 (100%)	125 (91%)	13 (9%)	11	39
2	F	137/138 (99%)	128 (93%)	9 (7%)	21	56
2	I	137/138 (99%)	128 (93%)	9 (7%)	21	56
All	All	2115/2190 (97%)	1903 (90%)	212 (10%)	9	34

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

Mol	Chain	Res	Type
1	A	2	LYS

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

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

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

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

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

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Mol	Chain	Res	Type
2	I	451	ASP

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	$\# Z > 2$
5	NAD	A	400	-	38,48,48	2.44	15 (39%)	47,73,73	2.95	23 (48%)
3	SUC	A	600	-	24,24,24	1.07	2 (8%)	36,36,36	0.63	1 (2%)
5	NAD	B	400	-	38,48,48	2.56	13 (34%)	47,73,73	3.12	17 (36%)
3	SUC	B	600	-	24,24,24	0.99	2 (8%)	36,36,36	0.67	1 (2%)
6	NDP	C	500	-	42,52,52	2.14	15 (35%)	55,80,80	2.80	24 (43%)
5	NAD	D	400	-	38,48,48	2.40	11 (28%)	47,73,73	2.99	21 (44%)
3	SUC	D	600	-	24,24,24	1.08	2 (8%)	36,36,36	0.70	1 (2%)
3	SUC	E	600	-	24,24,24	1.04	2 (8%)	36,36,36	0.71	1 (2%)
6	NDP	F	500	-	42,52,52	2.18	13 (30%)	55,80,80	2.62	19 (34%)
5	NAD	G	400	-	38,48,48	2.27	11 (28%)	47,73,73	3.13	23 (48%)
3	SUC	G	600	-	24,24,24	1.08	2 (8%)	36,36,36	0.70	1 (2%)
5	NAD	H	400	-	38,48,48	2.33	13 (34%)	47,73,73	2.64	18 (38%)
3	SUC	H	600	-	24,24,24	1.06	2 (8%)	36,36,36	0.69	1 (2%)
6	NDP	I	500	-	42,52,52	2.51	14 (33%)	55,80,80	2.59	18 (32%)

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
5	NAD	A	400	-	-	0/22/62/62	0/5/5/5
3	SUC	A	600	-	-	0/12/51/51	0/2/2/2
5	NAD	B	400	-	-	0/22/62/62	0/5/5/5
3	SUC	B	600	-	-	0/12/51/51	0/2/2/2
6	NDP	C	500	-	-	0/30/77/77	0/5/5/5
5	NAD	D	400	-	-	0/22/62/62	0/5/5/5
3	SUC	D	600	-	-	0/12/51/51	0/2/2/2
3	SUC	E	600	-	-	0/12/51/51	0/2/2/2
6	NDP	F	500	-	-	0/30/77/77	0/5/5/5
5	NAD	G	400	-	-	0/22/62/62	0/5/5/5
3	SUC	G	600	-	-	0/12/51/51	0/2/2/2
5	NAD	H	400	-	-	0/22/62/62	0/5/5/5
3	SUC	H	600	-	-	0/12/51/51	0/2/2/2
6	NDP	I	500	-	-	0/30/77/77	0/5/5/5

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	500	NDP	C4N-C5N	-4.96	1.38	1.49
6	I	500	NDP	C4N-C5N	-4.71	1.38	1.49
6	C	500	NDP	C4N-C5N	-4.42	1.39	1.49
3	E	600	SUC	C4'-C5'	-3.92	1.42	1.53
5	H	400	NAD	PN-O5D	-3.77	1.41	1.59
3	A	600	SUC	C4'-C5'	-3.71	1.43	1.53
3	D	600	SUC	C4'-C5'	-3.64	1.43	1.53
3	H	600	SUC	C4'-C5'	-3.36	1.44	1.53
3	G	600	SUC	C4'-C5'	-3.21	1.44	1.53
3	B	600	SUC	C4'-C5'	-3.21	1.44	1.53
6	C	500	NDP	P2B-O3X	-3.09	1.43	1.54
6	C	500	NDP	C3B-C2B	-3.05	1.46	1.53
6	I	500	NDP	C3B-C2B	-2.98	1.46	1.53
6	F	500	NDP	C3B-C4B	-2.96	1.45	1.53
5	D	400	NAD	C3B-C4B	-2.73	1.45	1.53
6	I	500	NDP	P2B-O3X	-2.68	1.45	1.54
6	I	500	NDP	O2B-C2B	-2.68	1.35	1.44
5	G	400	NAD	O2B-C2B	-2.68	1.36	1.43
5	D	400	NAD	O2B-C2B	-2.65	1.36	1.43
6	F	500	NDP	P2B-O3X	-2.62	1.45	1.54
5	A	400	NAD	PN-O2N	-2.60	1.43	1.54
6	F	500	NDP	C3B-C2B	-2.53	1.47	1.53
6	C	500	NDP	O2B-C2B	-2.53	1.36	1.44
6	I	500	NDP	P2B-O2X	-2.48	1.45	1.54
6	C	500	NDP	C3B-C4B	-2.47	1.46	1.53
5	G	400	NAD	C3B-C4B	-2.44	1.46	1.53
5	B	400	NAD	O2B-C2B	-2.44	1.37	1.43
5	D	400	NAD	C2B-C3B	-2.43	1.46	1.53
5	G	400	NAD	C2B-C3B	-2.40	1.46	1.53
5	B	400	NAD	C2B-C3B	-2.39	1.46	1.53
5	H	400	NAD	O2B-C2B	-2.39	1.37	1.43
5	A	400	NAD	O2B-C2B	-2.35	1.37	1.43
5	B	400	NAD	O5B-C5B	-2.32	1.35	1.44
6	I	500	NDP	C3B-C4B	-2.30	1.46	1.53
5	A	400	NAD	PN-O5D	-2.28	1.48	1.59
6	F	500	NDP	O2B-C2B	-2.27	1.37	1.44
5	H	400	NAD	C2B-C3B	-2.27	1.47	1.53
6	F	500	NDP	P2B-O2X	-2.26	1.46	1.54
5	A	400	NAD	PN-O1N	-2.21	1.43	1.51
5	H	400	NAD	C3B-C4B	-2.08	1.47	1.53
6	C	500	NDP	P2B-O2X	-2.07	1.47	1.54
5	B	400	NAD	C5B-C4B	-2.01	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	400	NAD	C2D-C3D	2.01	1.58	1.53
5	A	400	NAD	O3D-C3D	2.08	1.47	1.43
5	A	400	NAD	C2A-N3A	2.10	1.35	1.32
6	C	500	NDP	O3B-C3B	2.14	1.48	1.43
6	C	500	NDP	C2A-N1A	2.20	1.38	1.33
5	H	400	NAD	O3D-C3D	2.20	1.48	1.43
5	A	400	NAD	O3B-C3B	2.20	1.48	1.43
6	C	500	NDP	C1D-N1N	2.28	1.53	1.46
5	H	400	NAD	C2A-N3A	2.29	1.36	1.32
5	G	400	NAD	C2A-N3A	2.31	1.36	1.32
5	D	400	NAD	C2A-N3A	2.32	1.36	1.32
6	F	500	NDP	C6N-N1N	2.33	1.44	1.37
6	I	500	NDP	C2A-N3A	2.35	1.36	1.32
5	G	400	NAD	C2D-C3D	2.39	1.59	1.53
6	F	500	NDP	C2A-N1A	2.44	1.38	1.33
3	E	600	SUC	O5-C1	2.47	1.48	1.41
6	F	500	NDP	C6N-C5N	2.47	1.38	1.33
5	A	400	NAD	C4N-C3N	2.51	1.43	1.39
6	I	500	NDP	C6N-N1N	2.52	1.44	1.37
5	A	400	NAD	C2A-N1A	2.56	1.38	1.33
6	C	500	NDP	O4D-C1D	2.59	1.48	1.42
6	C	500	NDP	C6N-N1N	2.59	1.45	1.37
5	B	400	NAD	C2A-N1A	2.64	1.38	1.33
3	A	600	SUC	O5-C1	2.66	1.48	1.41
3	B	600	SUC	O5-C1	2.68	1.48	1.41
5	A	400	NAD	C2D-C3D	2.68	1.60	1.53
5	B	400	NAD	C2D-C3D	2.70	1.60	1.53
3	D	600	SUC	O5-C1	2.71	1.48	1.41
6	I	500	NDP	C2A-N1A	2.75	1.39	1.33
3	H	600	SUC	O5-C1	2.77	1.48	1.41
5	H	400	NAD	C2A-N1A	2.80	1.39	1.33
6	C	500	NDP	C6N-C5N	2.85	1.38	1.33
5	G	400	NAD	C2A-N1A	2.89	1.39	1.33
6	I	500	NDP	C6N-C5N	2.90	1.38	1.33
3	G	600	SUC	O5-C1	2.93	1.49	1.41
5	H	400	NAD	C4N-C3N	3.18	1.44	1.39
5	B	400	NAD	C4N-C3N	3.18	1.44	1.39
5	G	400	NAD	C4N-C3N	3.19	1.44	1.39
5	D	400	NAD	C2A-N1A	3.22	1.40	1.33
6	F	500	NDP	C2D-C1D	3.33	1.64	1.53
5	H	400	NAD	C2N-C3N	3.56	1.44	1.39
5	B	400	NAD	PN-O2N	3.58	1.70	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	500	NDP	C2N-C3N	3.59	1.43	1.34
5	D	400	NAD	C4N-C3N	3.63	1.45	1.39
5	A	400	NAD	C6N-N1N	3.65	1.45	1.35
5	D	400	NAD	C2N-C3N	3.77	1.44	1.39
5	D	400	NAD	C6N-N1N	3.95	1.46	1.35
5	A	400	NAD	C2N-C3N	3.97	1.45	1.39
5	H	400	NAD	C6N-N1N	4.06	1.46	1.35
6	C	500	NDP	C5A-C4A	4.14	1.49	1.40
6	F	500	NDP	C2N-C3N	4.21	1.45	1.34
6	I	500	NDP	C2N-C3N	4.33	1.45	1.34
5	G	400	NAD	C6N-N1N	4.34	1.47	1.35
5	D	400	NAD	O4D-C1D	4.35	1.46	1.41
5	B	400	NAD	C6N-N1N	4.38	1.47	1.35
5	B	400	NAD	C2N-C3N	4.48	1.45	1.39
5	B	400	NAD	O4D-C1D	4.61	1.47	1.41
5	G	400	NAD	C2N-C3N	4.67	1.46	1.39
5	A	400	NAD	C5A-C4A	4.87	1.51	1.40
6	F	500	NDP	C5A-C4A	5.00	1.51	1.40
6	I	500	NDP	C5A-C4A	5.16	1.52	1.40
5	B	400	NAD	C5A-C4A	5.18	1.52	1.40
5	G	400	NAD	C5A-C4A	5.19	1.52	1.40
5	H	400	NAD	C5A-C4A	5.20	1.52	1.40
5	D	400	NAD	C5A-C4A	5.55	1.53	1.40
5	A	400	NAD	O4D-C1D	5.59	1.48	1.41
6	F	500	NDP	O4B-C1B	6.36	1.49	1.41
6	C	500	NDP	O4B-C1B	6.73	1.49	1.41
6	I	500	NDP	O4B-C1B	6.84	1.49	1.41
5	G	400	NAD	O4B-C1B	7.42	1.50	1.41
6	I	500	NDP	O4D-C1D	7.77	1.61	1.42
5	D	400	NAD	O4B-C1B	7.85	1.51	1.41
5	A	400	NAD	O4B-C1B	7.99	1.51	1.41
5	H	400	NAD	O4B-C1B	8.11	1.51	1.41
5	B	400	NAD	O4B-C1B	8.44	1.51	1.41

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	400	NAD	C4D-O4D-C1D	-9.21	99.60	109.72
5	D	400	NAD	C4B-O4B-C1B	-8.59	100.28	109.72
5	G	400	NAD	C4D-O4D-C1D	-7.92	101.01	109.72
5	A	400	NAD	N3A-C2A-N1A	-7.51	123.14	128.89
6	I	500	NDP	C4B-O4B-C1B	-7.47	101.51	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	400	NAD	N3A-C2A-N1A	-7.43	123.21	128.89
5	A	400	NAD	O4D-C1D-N1N	-7.40	100.00	108.13
5	D	400	NAD	O4D-C1D-N1N	-7.38	100.03	108.13
5	G	400	NAD	C4B-O4B-C1B	-7.30	101.70	109.72
5	H	400	NAD	N3A-C2A-N1A	-7.23	123.36	128.89
6	C	500	NDP	N3A-C2A-N1A	-7.16	123.41	128.89
5	G	400	NAD	N3A-C2A-N1A	-7.03	123.51	128.89
6	C	500	NDP	C4B-O4B-C1B	-7.01	102.02	109.72
5	H	400	NAD	C4D-O4D-C1D	-6.97	102.06	109.72
5	A	400	NAD	C4B-O4B-C1B	-6.83	102.21	109.72
6	I	500	NDP	N3A-C2A-N1A	-6.60	123.84	128.89
5	H	400	NAD	C4B-O4B-C1B	-6.47	102.61	109.72
6	F	500	NDP	N3A-C2A-N1A	-6.45	123.96	128.89
6	C	500	NDP	O3-PN-O5D	-6.29	86.24	102.94
6	F	500	NDP	O3-PN-O5D	-6.24	86.39	102.94
5	D	400	NAD	O3-PN-O5D	-6.22	86.42	102.94
5	D	400	NAD	N3A-C2A-N1A	-6.02	124.29	128.89
5	B	400	NAD	O3-PN-O5D	-5.99	87.03	102.94
5	B	400	NAD	O4D-C1D-N1N	-5.93	101.62	108.13
5	D	400	NAD	C4D-O4D-C1D	-5.15	104.06	109.72
6	F	500	NDP	C4B-O4B-C1B	-5.08	104.14	109.72
5	A	400	NAD	C4D-O4D-C1D	-4.84	104.40	109.72
5	A	400	NAD	C3N-C7N-N7N	-4.70	112.68	117.82
5	G	400	NAD	C3N-C7N-N7N	-4.64	112.74	117.82
5	H	400	NAD	C3N-C7N-N7N	-4.44	112.96	117.82
5	B	400	NAD	C3N-C7N-N7N	-4.13	113.30	117.82
6	C	500	NDP	O4D-C1D-N1N	-4.00	99.63	108.07
6	I	500	NDP	C4D-O4D-C1D	-3.82	101.11	109.52
5	A	400	NAD	O3-PN-O5D	-3.50	93.65	102.94
5	D	400	NAD	C3N-C7N-N7N	-3.49	114.00	117.82
5	G	400	NAD	PN-O3-PA	-3.45	123.04	132.73
5	B	400	NAD	O3-PA-O5B	-3.34	94.07	102.94
6	F	500	NDP	O4D-C1D-N1N	-3.15	101.43	108.07
6	I	500	NDP	C2D-C3D-C4D	-3.14	96.15	102.61
6	C	500	NDP	C2D-C3D-C4D	-3.14	96.16	102.61
5	G	400	NAD	O4D-C1D-N1N	-3.09	104.74	108.13
5	H	400	NAD	O4D-C1D-N1N	-3.03	104.80	108.13
5	B	400	NAD	C4B-O4B-C1B	-2.97	106.46	109.72
5	A	400	NAD	PN-O3-PA	-2.91	124.56	132.73
6	I	500	NDP	PN-O3-PA	-2.81	124.83	132.73
5	A	400	NAD	C2D-C3D-C4D	-2.76	96.94	102.61
6	C	500	NDP	PN-O3-PA	-2.69	125.16	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	500	NDP	C4D-O4D-C1D	-2.66	103.66	109.52
5	G	400	NAD	C5D-C4D-C3D	-2.58	104.98	115.21
6	F	500	NDP	C4D-O4D-C1D	-2.56	103.89	109.52
6	C	500	NDP	O4B-C1B-N9A	-2.47	102.92	108.10
6	F	500	NDP	C3N-C2N-N1N	-2.40	119.70	123.14
5	G	400	NAD	O4B-C1B-N9A	-2.30	103.28	108.10
5	A	400	NAD	O4B-C4B-C3B	-2.25	100.61	105.15
3	E	600	SUC	C4-C3-C2	-2.22	106.64	110.79
5	G	400	NAD	O4B-C4B-C3B	-2.21	100.70	105.15
5	D	400	NAD	O4B-C4B-C3B	-2.20	100.71	105.15
3	H	600	SUC	C4-C3-C2	-2.16	106.76	110.79
3	D	600	SUC	C4-C3-C2	-2.16	106.76	110.79
3	G	600	SUC	C4-C3-C2	-2.15	106.77	110.79
6	I	500	NDP	O4B-C4B-C3B	-2.15	100.82	105.15
6	F	500	NDP	C2D-C3D-C4D	-2.14	98.21	102.61
3	A	600	SUC	C4-C3-C2	-2.14	106.80	110.79
5	H	400	NAD	O4B-C4B-C3B	-2.12	100.88	105.15
5	D	400	NAD	O4B-C1B-N9A	-2.10	103.69	108.10
6	C	500	NDP	O4B-C4B-C3B	-2.07	100.98	105.15
5	G	400	NAD	O4D-C4D-C5D	-2.07	101.93	109.32
6	I	500	NDP	C3N-C2N-N1N	-2.06	120.19	123.14
5	D	400	NAD	C2D-C3D-C4D	-2.06	98.39	102.61
6	C	500	NDP	C1B-N9A-C4A	-2.05	123.85	126.94
6	F	500	NDP	O4B-C1B-N9A	-2.03	103.84	108.10
3	B	600	SUC	C4-C3-C2	-2.02	107.02	110.79
6	F	500	NDP	C2A-N1A-C6A	2.01	122.35	118.77
5	A	400	NAD	C2A-N1A-C6A	2.02	122.37	118.77
5	D	400	NAD	O4D-C4D-C5D	2.02	116.54	109.32
5	H	400	NAD	O5D-C5D-C4D	2.05	116.67	109.12
5	G	400	NAD	O2D-C2D-C3D	2.05	118.51	111.83
5	A	400	NAD	O4D-C4D-C5D	2.06	116.70	109.32
6	C	500	NDP	O2D-C2D-C3D	2.08	118.59	111.83
5	D	400	NAD	C2N-C3N-C4N	2.10	120.62	118.29
5	H	400	NAD	C2A-N1A-C6A	2.10	122.51	118.77
5	D	400	NAD	O5D-PN-O1N	2.11	117.80	109.62
5	B	400	NAD	C2A-N1A-C6A	2.11	122.55	118.77
6	I	500	NDP	C3D-C2D-C1D	2.12	105.66	101.40
6	C	500	NDP	C2A-N1A-C6A	2.13	122.57	118.77
5	G	400	NAD	O7N-C7N-C3N	2.15	121.94	119.59
5	G	400	NAD	C2N-C3N-C4N	2.22	120.76	118.29
6	I	500	NDP	O2D-C2D-C3D	2.23	119.09	111.83
5	H	400	NAD	C2B-C1B-N9A	2.29	117.80	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	400	NAD	O5D-PN-O1N	2.31	118.58	109.62
5	H	400	NAD	C5N-C6N-N1N	2.32	124.48	120.47
5	H	400	NAD	O7N-C7N-N7N	2.33	125.87	122.59
5	A	400	NAD	O4B-C4B-C5B	2.34	117.68	109.32
5	D	400	NAD	C5N-C6N-N1N	2.34	124.52	120.47
6	C	500	NDP	O4D-C4D-C5D	2.35	117.74	109.32
6	I	500	NDP	C5N-C4N-C3N	2.36	119.02	112.52
5	B	400	NAD	C2N-C3N-C4N	2.36	120.92	118.29
6	C	500	NDP	O3D-C3D-C4D	2.37	118.15	111.05
6	F	500	NDP	O4B-C4B-C5B	2.38	117.83	109.32
5	A	400	NAD	O2D-C2D-C3D	2.39	119.61	111.83
6	C	500	NDP	C5N-C4N-C3N	2.40	119.12	112.52
6	F	500	NDP	O5D-PN-O1N	2.42	119.02	109.62
6	F	500	NDP	C5N-C4N-C3N	2.44	119.24	112.52
5	A	400	NAD	O7N-C7N-N7N	2.44	126.03	122.59
5	H	400	NAD	C2N-C3N-C4N	2.47	121.04	118.29
6	C	500	NDP	O5D-PN-O1N	2.53	119.42	109.62
5	A	400	NAD	C5N-C6N-N1N	2.58	124.94	120.47
5	B	400	NAD	C5N-C6N-N1N	2.59	124.95	120.47
5	G	400	NAD	O3-PN-O5D	2.59	109.81	102.94
6	I	500	NDP	O3D-C3D-C4D	2.59	118.83	111.05
5	B	400	NAD	O3D-C3D-C4D	2.60	118.84	111.05
6	C	500	NDP	O4B-C4B-C5B	2.60	118.63	109.32
5	G	400	NAD	C5N-C6N-N1N	2.60	124.97	120.47
6	C	500	NDP	C2D-C1D-N1N	2.62	120.41	113.34
5	G	400	NAD	O4B-C4B-C5B	2.68	118.91	109.32
6	I	500	NDP	O4B-C4B-C5B	2.71	119.00	109.32
5	A	400	NAD	C2N-C3N-C4N	2.73	121.32	118.29
5	H	400	NAD	O4B-C4B-C5B	2.74	119.12	109.32
5	G	400	NAD	O3D-C3D-C4D	2.75	119.31	111.05
5	A	400	NAD	O3D-C3D-C4D	2.82	119.51	111.05
6	F	500	NDP	O3D-C3D-C4D	2.89	119.73	111.05
5	H	400	NAD	O3D-C3D-C4D	3.03	120.14	111.05
5	D	400	NAD	O3D-C3D-C4D	3.08	120.29	111.05
6	C	500	NDP	O2B-C2B-C3B	3.18	123.89	111.51
5	D	400	NAD	O4B-C4B-C5B	3.28	121.04	109.32
6	I	500	NDP	C2B-C3B-C4B	3.31	109.68	101.85
6	I	500	NDP	O2B-C2B-C3B	3.36	124.59	111.51
5	A	400	NAD	C2B-C1B-N9A	3.37	119.44	114.29
5	B	400	NAD	O4D-C4D-C3D	3.44	112.08	105.15
6	C	500	NDP	O4D-C4D-C3D	3.44	112.09	105.15
5	D	400	NAD	O5B-C5B-C4B	3.46	121.86	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	400	NAD	C2B-C3B-C4B	3.57	109.94	102.61
6	C	500	NDP	C2B-C3B-C4B	3.60	110.39	101.85
5	G	400	NAD	O5B-C5B-C4B	3.68	122.68	109.12
5	D	400	NAD	O2B-C2B-C3B	3.75	124.01	111.83
5	A	400	NAD	O5B-C5B-C4B	3.76	122.98	109.12
6	F	500	NDP	O2B-C2B-C3B	3.79	126.24	111.51
5	A	400	NAD	C2B-C3B-C4B	3.81	110.44	102.61
5	H	400	NAD	O5B-C5B-C4B	3.92	123.56	109.12
5	G	400	NAD	C2B-C3B-C4B	3.92	110.67	102.61
5	H	400	NAD	C2B-C3B-C4B	3.95	110.73	102.61
5	D	400	NAD	O5D-C5D-C4D	3.96	123.72	109.12
6	C	500	NDP	O5D-C5D-C4D	4.00	123.87	109.12
6	F	500	NDP	O5B-C5B-C4B	4.00	123.87	109.12
6	F	500	NDP	O5D-C5D-C4D	4.05	124.04	109.12
6	F	500	NDP	C2B-C3B-C4B	4.10	111.55	101.85
5	G	400	NAD	O2B-C2B-C3B	4.11	125.21	111.83
5	A	400	NAD	O5D-C5D-C4D	4.11	124.28	109.12
6	I	500	NDP	O5B-C5B-C4B	4.13	124.34	109.12
6	F	500	NDP	O4D-C4D-C3D	4.14	113.48	105.15
6	I	500	NDP	C2D-C1D-N1N	4.14	124.53	113.34
6	C	500	NDP	O5B-C5B-C4B	4.21	124.65	109.12
5	G	400	NAD	C2B-C1B-N9A	4.23	120.76	114.29
6	I	500	NDP	O4D-C4D-C3D	4.26	113.72	105.15
5	B	400	NAD	C2B-C3B-C4B	4.44	111.74	102.61
5	G	400	NAD	O4D-C4D-C3D	4.46	114.12	105.15
5	B	400	NAD	O2B-C2B-C3B	4.48	126.39	111.83
5	H	400	NAD	O2B-C2B-C3B	4.57	126.68	111.83
5	D	400	NAD	O4D-C4D-C3D	4.62	114.46	105.15
5	A	400	NAD	O4D-C4D-C3D	4.73	114.68	105.15
5	A	400	NAD	O2B-C2B-C3B	4.74	127.26	111.83
5	D	400	NAD	C2B-C1B-N9A	4.75	121.56	114.29
5	H	400	NAD	O4D-C4D-C3D	5.12	115.47	105.15
5	B	400	NAD	O5D-C5D-C4D	5.48	129.33	109.12
5	B	400	NAD	O4B-C4B-C5B	7.91	137.60	109.32
6	I	500	NDP	P2B-O2B-C2B	9.10	143.39	121.56
5	G	400	NAD	O5D-C5D-C4D	9.13	142.78	109.12
6	F	500	NDP	P2B-O2B-C2B	9.30	143.87	121.56
6	C	500	NDP	P2B-O2B-C2B	9.59	144.55	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	400	NAD	2	0
5	B	400	NAD	9	0
3	B	600	SUC	1	0
6	C	500	NDP	4	0
5	D	400	NAD	3	0
6	F	500	NDP	10	0
5	G	400	NAD	6	0
5	H	400	NAD	8	0
3	H	600	SUC	1	0
6	I	500	NDP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.18	2 (0%) 90 80	30, 51, 77, 102	0
1	B	359/384 (93%)	-0.21	0 100 100	28, 52, 72, 98	0
1	D	378/384 (98%)	0.03	10 (2%) 59 35	36, 68, 94, 104	0
1	E	359/384 (93%)	-0.17	4 (1%) 82 66	33, 60, 79, 91	0
1	G	364/384 (94%)	-0.19	1 (0%) 94 88	35, 59, 84, 102	0
1	H	357/384 (92%)	0.09	10 (2%) 56 32	39, 72, 96, 104	0
2	C	174/174 (100%)	-0.38	0 100 100	32, 47, 61, 68	0
2	F	173/174 (99%)	-0.34	0 100 100	40, 52, 63, 75	0
2	I	173/174 (99%)	-0.25	0 100 100	42, 58, 73, 79	0
All	All	2700/2826 (95%)	-0.15	27 (1%) 84 69	28, 57, 90, 104	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.9
1	H	96	LEU	3.4
1	D	225	ALA	3.4
1	H	64	ALA	3.3
1	D	226	MET	3.1
1	D	371	ASP	3.1
1	D	224	GLU	3.1
1	E	30	GLY	3.0
1	H	81	GLU	2.6
1	H	1	MET	2.6
1	D	116	LYS	2.6
1	H	268	PRO	2.5
1	E	1	MET	2.5
1	D	230	GLU	2.4
1	E	245	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	78	MET	2.3
1	H	71	VAL	2.3
1	H	368	VAL	2.2
1	D	81	GLU	2.2
1	G	220	THR	2.2
1	H	267	ILE	2.2
1	D	353	THR	2.2
1	H	349	LYS	2.1
1	A	222	ASP	2.1
1	A	243	PHE	2.1
1	E	348	ASP	2.1
1	D	372	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	SUC	H	600	23/23	0.86	0.38	7.83	82,84,85,87	0
3	SUC	G	600	23/23	0.73	0.43	5.71	97,99,99,99	0
3	SUC	B	600	23/23	0.76	0.31	4.72	84,88,89,89	0
3	SUC	E	600	23/23	0.86	0.25	3.39	70,75,77,77	0
5	NAD	B	400	44/44	0.75	0.35	3.09	104,104,105,105	0
3	SUC	D	600	23/23	0.86	0.28	2.29	79,82,83,83	0
3	SUC	A	600	23/23	0.88	0.22	0.98	70,75,78,79	0
4	NA	A	601	1/1	0.87	0.24	0.65	50,50,50,50	0
5	NAD	G	400	44/44	0.90	0.24	0.63	65,72,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAD	H	400	44/44	0.85	0.28	0.18	88,90,99,101	0
5	NAD	A	400	44/44	0.91	0.21	0.17	65,71,75,75	0
5	NAD	D	400	44/44	0.93	0.20	-0.15	54,60,64,65	0
4	NA	D	602	1/1	0.92	0.19	-0.38	69,69,69,69	0
6	NDP	C	500	48/48	0.95	0.17	-0.47	38,40,44,46	0
6	NDP	F	500	48/48	0.94	0.18	-0.55	48,52,56,58	0
6	NDP	I	500	48/48	0.92	0.17	-0.99	56,58,64,64	0
4	NA	G	603	1/1	0.95	0.10	-3.54	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.