Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:23 PM GMT

PDB ID	:	1K0U
Title	:	Inhibition of S-adenosylhomocysteine Hydrolase by "acyclic sugar" Adenosine Analogue D-eritadenine
Authors	:	Takusagawa, F.; Huang, Y.; Komoto, J.; Takata, Y.; Gomi, T.; Ogawa, H.; Fujioka, M.; Powell, D.
Deposited on	:	2001-09-20
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

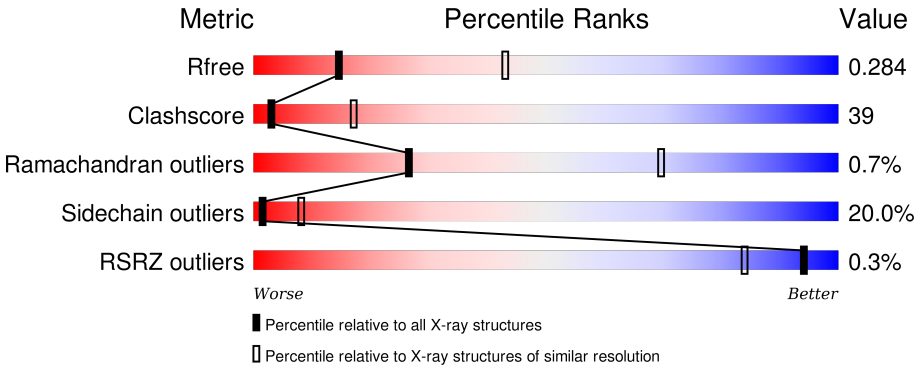
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	47% 41% 11%
1	B	431	46% 43% 10%
1	C	431	49% 41% 9%
1	D	431	46% 42% 11%
1	E	431	35% 52% 13%

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Mol	Chain	Length	Quality of chain
1	F	431	37% 52% 11%
1	G	431	34% 52% 13%
1	H	431	35% 50% 15%

2 Entry composition (i)

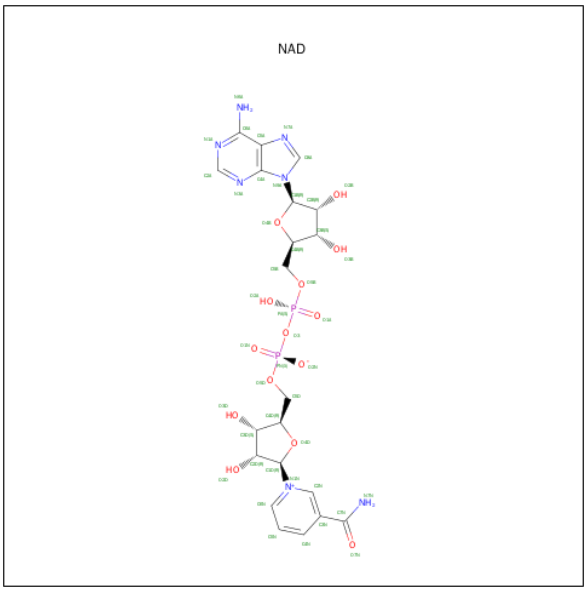
There are 4 unique types of molecules in this entry. The entry contains 27522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE.

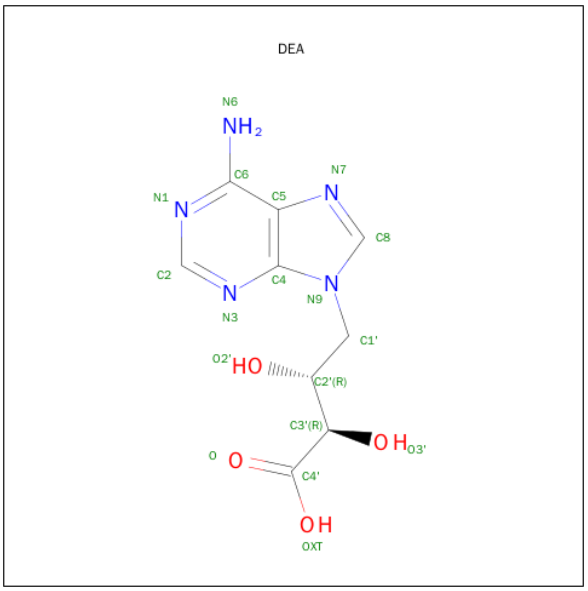
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	B	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	C	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	D	430	Total	C	N	O	S	0	0	0
			3319	2108	571	615	25			
1	E	430	Total	C	N	O	S	0	0	0
	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

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is D-ERITADENINE (three-letter code: DEA) (formula: $C_9H_{11}N_5O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 18 9 5 4	0	0
3	B	1	Total C N O 18 9 5 4	0	0
3	C	1	Total C N O 18 9 5 4	0	0
3	D	1	Total C N O 18 9 5 4	0	0
3	E	1	Total C N O 18 9 5 4	0	0
3	F	1	Total C N O 18 9 5 4	0	0
3	G	1	Total C N O 18 9 5 4	0	0
3	H	1	Total C N O 18 9 5 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	B	52	Total O 52 52	0	0
4	C	53	Total O 53 53	0	0
4	D	51	Total O 51 51	0	0

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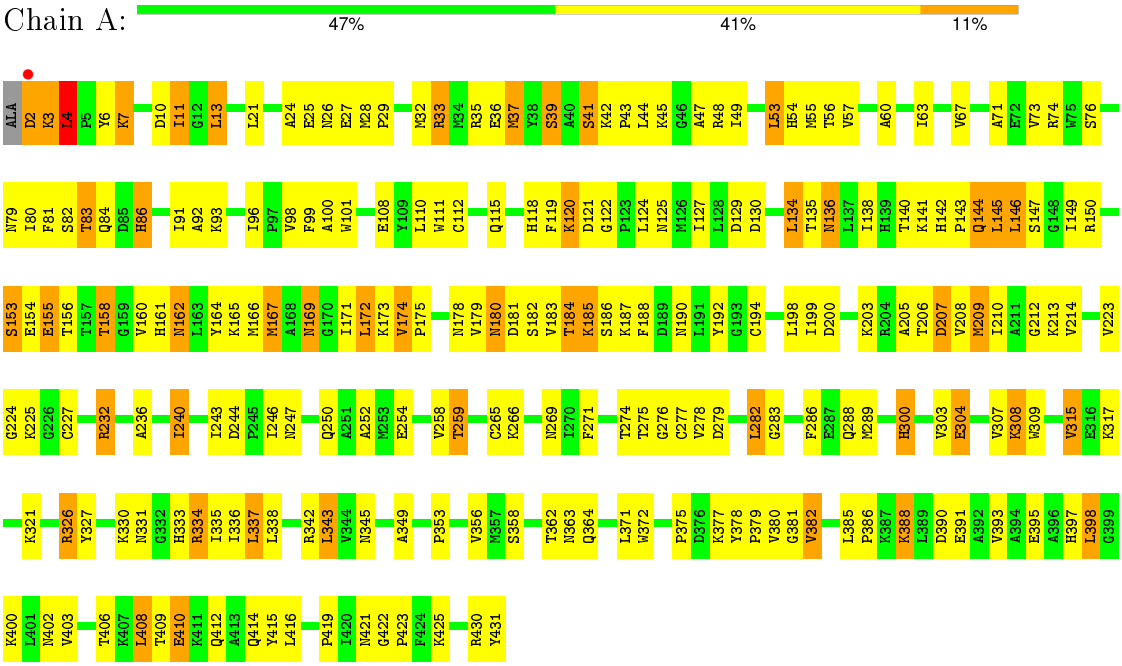
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	68	Total O 68 68	0	0
4	F	68	Total O 68 68	0	0
4	G	57	Total O 57 57	0	0
4	H	56	Total O 56 56	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

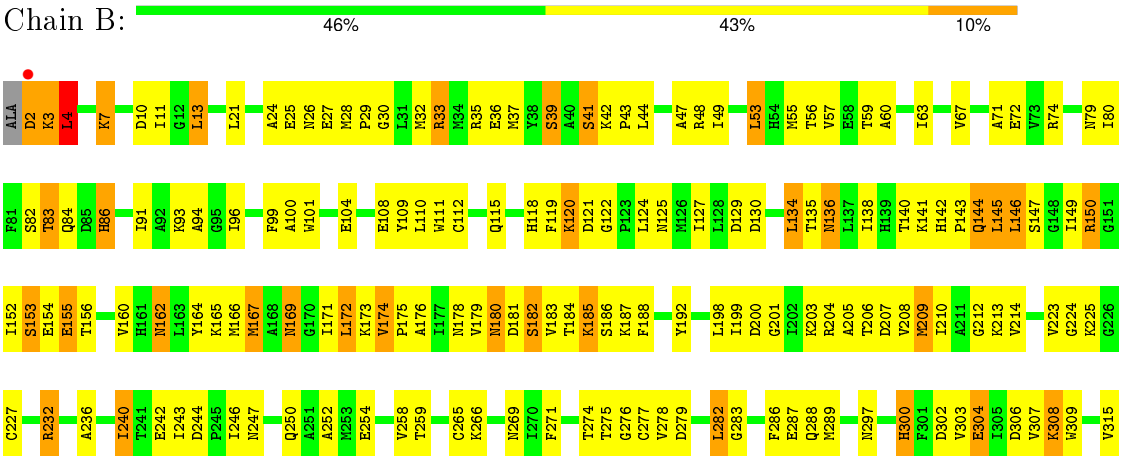
- Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

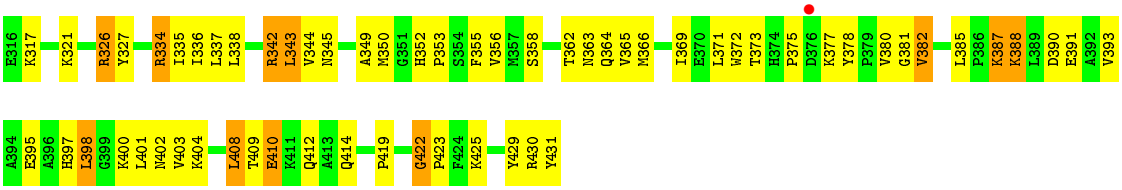
Chain A:



- Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

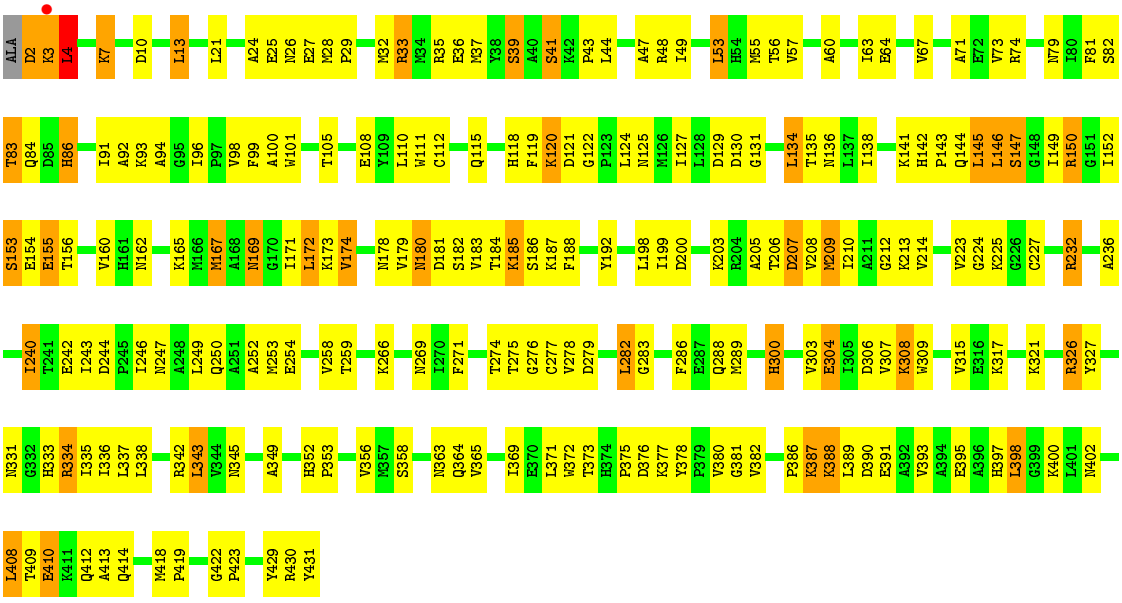
Chain B:





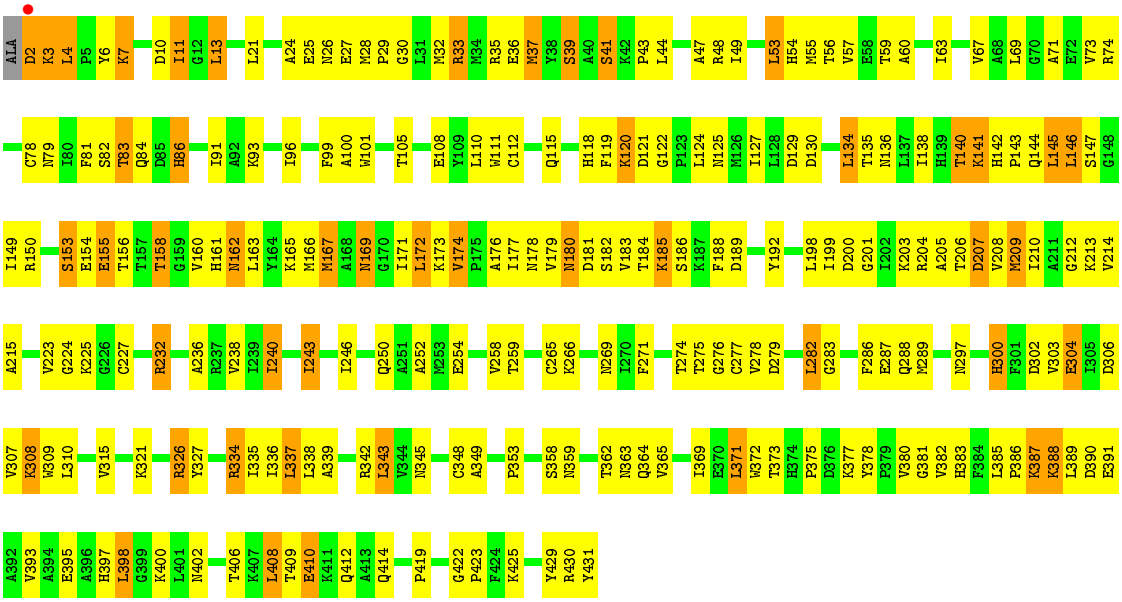
• Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

Chain C:



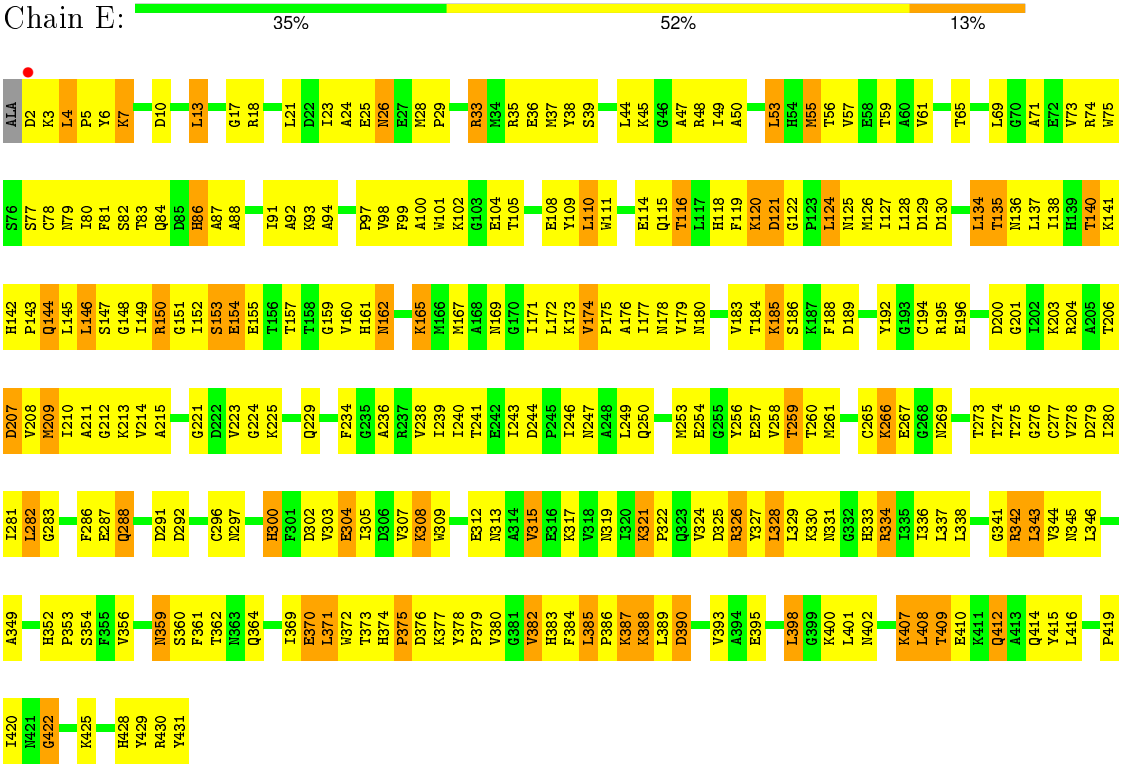
• Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

Chain D:



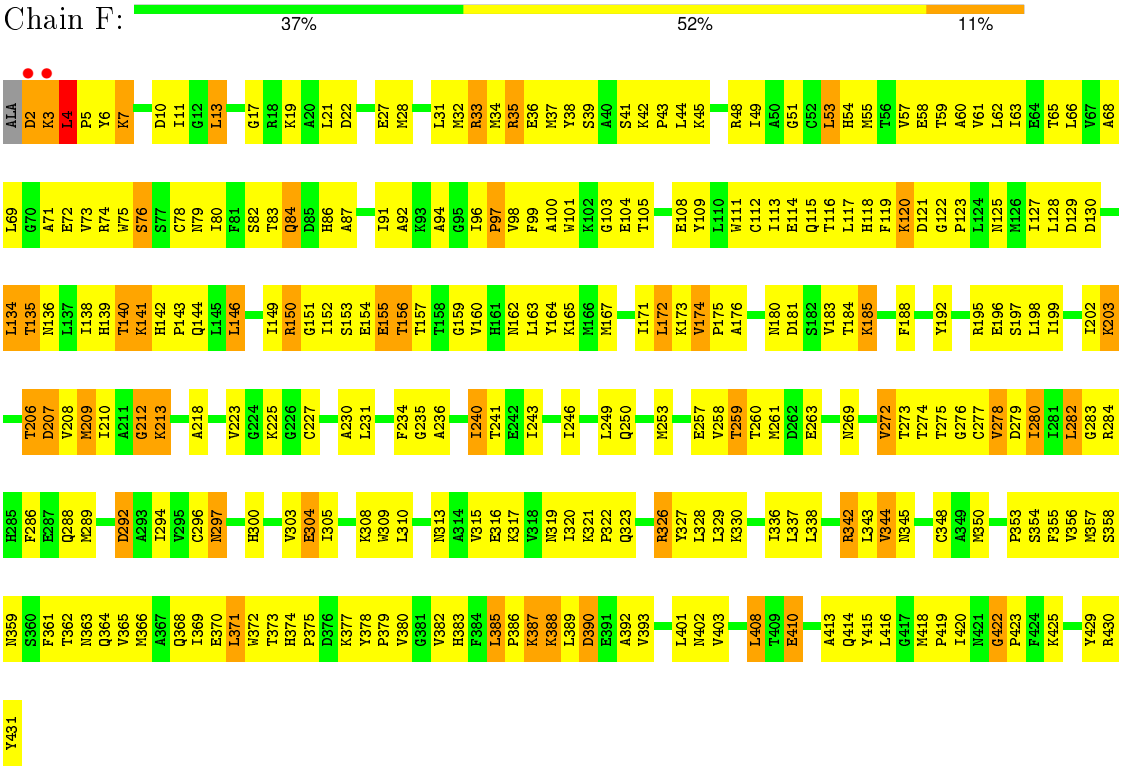
• Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

Chain E:



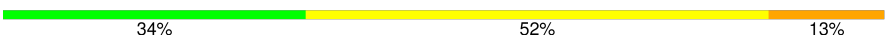
• Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

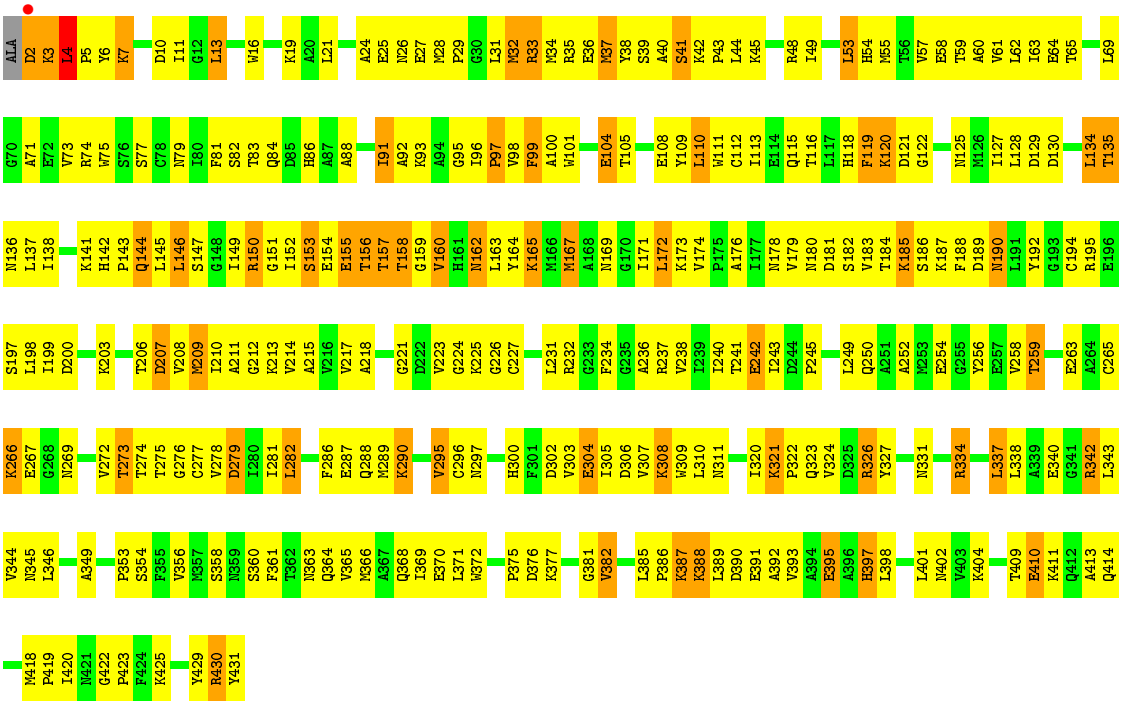
Chain F:



• Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

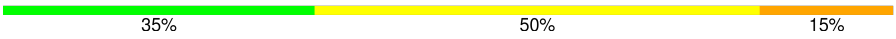
Chain G:

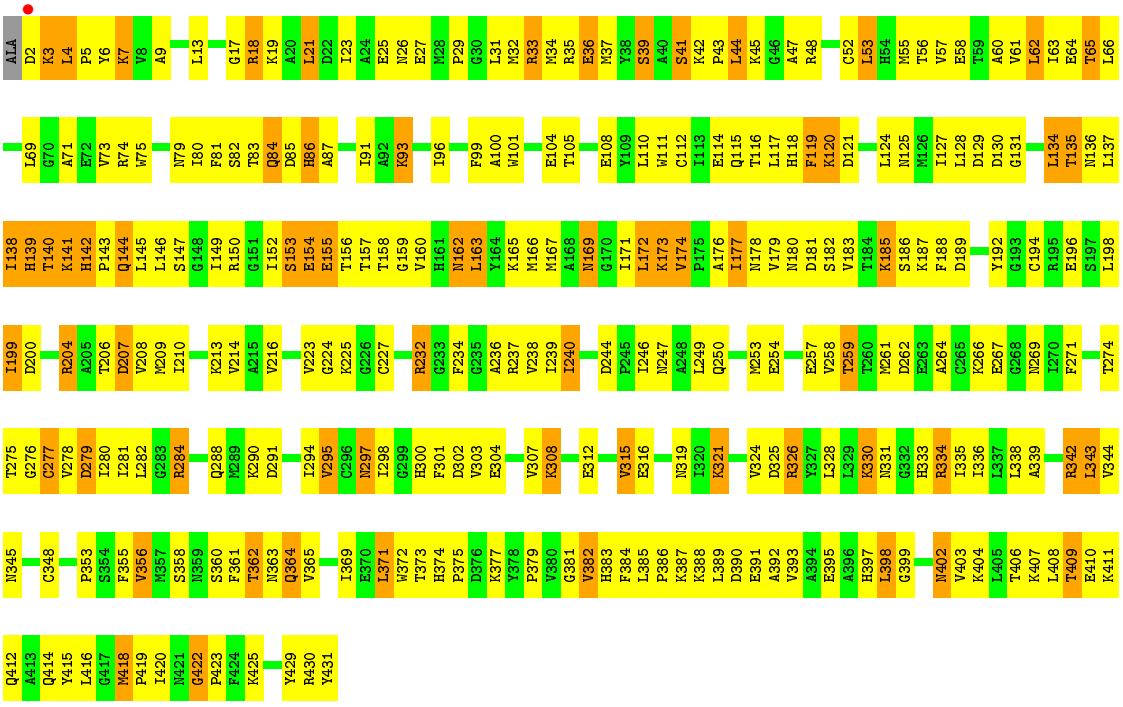




• Molecule 1: S-ADENOSYL-L-HOMOCYSTEINE HYDROLASE

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.87Å 177.37Å 112.16Å 90.00° 107.60° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 91.56 – 2.99	Depositor EDS
% Data completeness (in resolution range)	85.0 (10.00-3.00) 87.4 (91.56-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.183 , 0.265 0.198 , 0.284	Depositor DCC
R_{free} test set	4935 reflections (8.36%)	DCC
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 59048 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	27522	wwPDB-VP
Average B, all atoms (Å^2)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: DEA, NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/3384	0.55	0/4579
1	B	0.33	0/3384	0.55	0/4579
1	C	0.33	0/3384	0.54	0/4579
1	D	0.33	0/3384	0.55	0/4579
1	E	0.33	0/3384	0.59	0/4579
1	F	0.33	0/3384	0.59	0/4579
1	G	0.34	0/3384	0.58	0/4579
1	H	0.35	0/3384	0.61	0/4579
All	All	0.33	0/27072	0.57	0/36632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3319	0	3341	242	0
1	B	3319	0	3341	246	0
1	C	3319	0	3341	230	0
1	D	3319	0	3341	238	0
1	E	3319	0	3341	305	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3319	0	3341	284	0
1	G	3319	0	3341	341	0
1	H	3319	0	3341	324	0
2	A	44	0	26	2	0
2	B	44	0	26	3	0
2	C	44	0	26	3	0
2	D	44	0	26	2	0
2	E	44	0	26	3	0
2	F	44	0	26	2	0
2	G	44	0	26	6	0
2	H	44	0	26	5	0
3	A	18	0	10	0	0
3	B	18	0	10	0	0
3	C	18	0	10	0	0
3	D	18	0	10	0	0
3	E	18	0	10	0	0
3	F	18	0	10	1	0
3	G	18	0	10	0	0
3	H	18	0	10	0	0
4	A	69	0	0	0	0
4	B	52	0	0	1	0
4	C	53	0	0	0	0
4	D	51	0	0	0	0
4	E	68	0	0	0	0
4	F	68	0	0	0	0
4	G	57	0	0	0	0
4	H	56	0	0	0	0
All	All	27522	0	27016	2082	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 39.

All (2082) 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:33:ARG:HE	1:H:33:ARG:HA	0.99	1.13
1:D:33:ARG:HH21	1:D:36:GLU:HB2	1.17	1.09
1:F:150:ARG:HD3	1:F:375:PRO:HB3	1.33	1.09
1:F:33:ARG:HG3	1:F:33:ARG:HH11	0.95	1.09
1:H:33:ARG:NE	1:H:33:ARG:HA	1.64	1.07
1:E:3:LYS:HD3	1:E:115:GLN:HE22	0.96	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ASP:HB3	1:F:13:LEU:HD22	1.38	1.05
1:H:120:LYS:HE2	1:H:120:LYS:H	1.23	1.04
1:H:33:ARG:HH22	1:H:37:MET:N	1.55	1.03
1:H:408:LEU:HD21	1:H:416:LEU:HD12	1.36	1.02
1:F:278:VAL:HG12	1:F:303:VAL:HB	1.41	1.01
1:E:395:GLU:HA	1:E:398:LEU:HD22	1.43	1.00
1:E:3:LYS:HD3	1:E:115:GLN:NE2	1.77	0.99
1:C:33:ARG:HH21	1:C:36:GLU:HB2	1.23	0.99
1:C:395:GLU:HA	1:C:398:LEU:HD22	1.44	0.99
1:B:353:PRO:HB2	1:D:209:MET:HB2	1.44	0.99
1:D:120:LYS:H	1:D:120:LYS:HE2	1.27	0.99
1:H:386:PRO:HG2	1:H:389:LEU:HD12	1.45	0.99
1:G:33:ARG:HH21	1:G:36:GLU:HB2	1.23	0.98
1:E:195:ARG:HH11	1:E:229:GLN:HE22	1.10	0.97
1:H:278:VAL:HG12	1:H:303:VAL:HB	1.47	0.97
1:A:33:ARG:HH21	1:A:36:GLU:HB2	1.29	0.96
1:B:180:ASN:HA	1:B:185:LYS:HE3	1.48	0.96
1:F:33:ARG:HG3	1:F:33:ARG:NH1	1.76	0.95
1:E:195:ARG:NH1	1:E:229:GLN:HE22	1.64	0.95
1:G:275:THR:HG22	1:G:277:CYS:H	1.31	0.94
1:B:7:LYS:HZ3	1:B:101:TRP:HE3	1.00	0.94
1:B:33:ARG:HH21	1:B:36:GLU:HB2	1.33	0.94
1:A:7:LYS:HZ3	1:A:101:TRP:HE3	1.02	0.94
1:B:275:THR:HG22	1:B:277:CYS:H	1.29	0.94
1:H:33:ARG:NH2	1:H:37:MET:H	1.64	0.94
1:C:7:LYS:HZ3	1:C:101:TRP:HE3	1.02	0.93
1:H:33:ARG:HH22	1:H:37:MET:H	0.96	0.93
1:C:275:THR:HG22	1:C:277:CYS:H	1.31	0.93
1:D:7:LYS:HZ3	1:D:101:TRP:HE3	0.93	0.92
1:F:57:VAL:H	1:F:84:GLN:NE2	1.67	0.92
1:B:120:LYS:H	1:B:120:LYS:HE2	1.36	0.91
1:E:277:CYS:HB2	1:F:416:LEU:HD21	1.52	0.91
1:E:275:THR:HG22	1:E:277:CYS:H	1.35	0.91
1:F:7:LYS:HZ3	1:F:101:TRP:HE3	0.93	0.91
1:E:315:VAL:HG23	1:E:330:LYS:HG2	1.49	0.91
1:H:55:MET:HB3	1:H:83:THR:HG23	1.53	0.91
1:E:120:LYS:HE2	1:E:120:LYS:H	1.35	0.91
1:G:321:LYS:HD3	1:G:324:VAL:HG21	1.54	0.90
1:H:7:LYS:NZ	1:H:101:TRP:HE3	1.70	0.90
1:E:136:ASN:O	1:E:140:THR:HG23	1.71	0.90
1:E:195:ARG:HH11	1:E:229:GLN:NE2	1.68	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:LEU:HD13	1:F:99:PHE:HE1	1.34	0.90
1:B:395:GLU:HA	1:B:398:LEU:HD22	1.51	0.89
1:A:55:MET:HB3	1:A:83:THR:HG23	1.53	0.89
1:E:209:MET:HB2	1:G:353:PRO:HB2	1.55	0.89
1:D:55:MET:HB3	1:D:83:THR:HG23	1.55	0.89
1:F:275:THR:HG22	1:F:277:CYS:H	1.37	0.88
1:E:258:VAL:HB	1:F:403:VAL:HG13	1.53	0.88
1:B:55:MET:HB3	1:B:83:THR:HG23	1.56	0.88
1:A:395:GLU:HA	1:A:398:LEU:HD22	1.54	0.88
1:C:430:ARG:HD3	1:D:430:ARG:HA	1.53	0.88
1:G:7:LYS:NZ	1:G:101:TRP:HE3	1.70	0.88
1:H:419:PRO:HB2	1:H:422:GLY:H	1.38	0.87
1:E:35:ARG:HG3	1:E:65:THR:HG23	1.54	0.87
1:E:353:PRO:HB2	1:G:209:MET:HB2	1.55	0.87
1:E:244:ASP:HB3	1:E:247:ASN:HB2	1.54	0.87
1:F:198:LEU:HD22	1:F:227:CYS:HB3	1.55	0.87
1:E:150:ARG:HD3	1:E:375:PRO:HB3	1.55	0.87
1:A:53:LEU:HD12	1:A:130:ASP:HB2	1.56	0.87
1:D:395:GLU:HA	1:D:398:LEU:HD22	1.54	0.87
1:A:120:LYS:H	1:A:120:LYS:HE2	1.37	0.86
1:C:120:LYS:HE2	1:C:120:LYS:H	1.37	0.86
1:A:37:MET:HB3	1:H:284:ARG:NH2	1.90	0.86
1:A:275:THR:HG22	1:A:277:CYS:H	1.38	0.86
1:G:395:GLU:HA	1:G:398:LEU:HD13	1.56	0.86
1:D:21:LEU:HD12	1:D:57:VAL:HG13	1.57	0.86
1:H:33:ARG:NE	1:H:33:ARG:CA	2.39	0.86
1:E:214:VAL:H	1:E:269:ASN:HD22	1.22	0.86
1:F:55:MET:HB3	1:F:83:THR:HG23	1.58	0.85
1:A:209:MET:HB2	1:C:353:PRO:HB2	1.58	0.85
1:F:33:ARG:HH11	1:F:33:ARG:CG	1.86	0.85
1:B:33:ARG:HG3	1:B:33:ARG:HH11	1.41	0.85
1:E:3:LYS:CD	1:E:115:GLN:HE22	1.87	0.85
1:C:430:ARG:HA	1:D:430:ARG:HD3	1.57	0.85
1:H:198:LEU:HD22	1:H:227:CYS:HB3	1.58	0.85
1:H:7:LYS:HZ3	1:H:101:TRP:HE3	0.87	0.85
1:G:33:ARG:HG3	1:G:33:ARG:HH11	1.41	0.84
1:C:150:ARG:HD3	1:C:375:PRO:HB3	1.57	0.84
1:E:7:LYS:NZ	1:E:101:TRP:HE3	1.76	0.84
1:A:326:ARG:HD2	1:A:336:ILE:HG12	1.60	0.84
1:G:55:MET:HB3	1:G:83:THR:HG23	1.60	0.83
1:E:33:ARG:NE	1:E:33:ARG:HA	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:HA	1:A:185:LYS:HE3	1.59	0.83
1:E:153:SER:HB3	1:E:364:GLN:HE22	1.43	0.83
1:F:4:LEU:N	1:F:4:LEU:HD12	1.94	0.83
1:F:54:HIS:HB3	1:F:82:SER:HB2	1.59	0.83
1:D:7:LYS:NZ	1:D:101:TRP:HE3	1.76	0.83
1:F:57:VAL:HG23	1:F:84:GLN:NE2	1.93	0.83
1:A:10:ASP:HB3	1:A:13:LEU:HD22	1.61	0.83
1:H:277:CYS:HB3	1:H:280:ILE:HD11	1.61	0.83
1:F:57:VAL:HG23	1:F:84:GLN:HE21	1.43	0.82
1:F:7:LYS:NZ	1:F:101:TRP:HE3	1.76	0.82
1:F:326:ARG:HH11	1:F:326:ARG:HG2	1.41	0.82
1:B:10:ASP:HB3	1:B:13:LEU:HD22	1.62	0.82
1:G:4:LEU:HD12	1:G:4:LEU:N	1.95	0.82
1:C:53:LEU:HD12	1:C:130:ASP:HB2	1.62	0.81
1:E:55:MET:HB3	1:E:83:THR:HG23	1.59	0.81
1:G:277:CYS:HB2	1:H:416:LEU:HD21	1.63	0.81
1:D:33:ARG:NH2	1:D:36:GLU:HB2	1.95	0.81
1:A:37:MET:HB3	1:H:284:ARG:HH21	1.44	0.81
1:G:13:LEU:HB3	1:G:86:HIS:HA	1.63	0.81
1:D:275:THR:HG22	1:D:277:CYS:H	1.45	0.81
1:H:7:LYS:HE2	1:H:112:CYS:SG	2.21	0.81
1:H:244:ASP:HB3	1:H:247:ASN:HD22	1.45	0.81
1:H:21:LEU:O	1:H:25:GLU:HG3	1.81	0.81
1:E:369:ILE:O	1:E:373:THR:HB	1.81	0.80
1:B:150:ARG:HD3	1:B:375:PRO:HB3	1.63	0.80
1:C:55:MET:HB3	1:C:83:THR:HG23	1.62	0.80
1:A:430:ARG:HD3	1:B:430:ARG:HA	1.62	0.80
1:G:295:VAL:HG13	1:G:305:ILE:HD13	1.62	0.80
1:G:7:LYS:HZ3	1:G:101:TRP:HE3	0.84	0.80
1:G:275:THR:HG22	1:G:276:GLY:N	1.96	0.80
1:F:209:MET:SD	1:H:353:PRO:HG2	2.22	0.80
1:D:7:LYS:HE2	1:D:112:CYS:SG	2.22	0.79
1:C:7:LYS:NZ	1:C:101:TRP:HE3	1.79	0.79
1:H:41:SER:HB2	1:H:43:PRO:HD3	1.63	0.79
1:H:2:ASP:OD2	1:H:118:HIS:HB2	1.81	0.79
1:B:3:LYS:HD2	1:B:115:GLN:OE1	1.83	0.79
1:D:53:LEU:HD12	1:D:130:ASP:HB2	1.64	0.79
1:B:7:LYS:HZ1	1:B:100:ALA:N	1.80	0.79
1:G:300:HIS:HA	1:G:343:LEU:HD11	1.65	0.79
1:A:353:PRO:HB2	1:C:209:MET:HB2	1.64	0.79
1:B:53:LEU:HD12	1:B:130:ASP:HB2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:GLY:HA3	1:F:371:LEU:HG	1.66	0.78
1:G:430:ARG:HD3	1:H:430:ARG:HA	1.64	0.78
1:D:2:ASP:HB2	1:D:74:ARG:HH12	1.49	0.78
1:F:326:ARG:HD2	1:F:336:ILE:HG12	1.66	0.78
1:H:225:LYS:NZ	1:H:250:GLN:HE22	1.81	0.78
1:C:180:ASN:HA	1:C:185:LYS:HE3	1.66	0.77
1:D:180:ASN:HA	1:D:185:LYS:HE3	1.66	0.77
1:A:430:ARG:HA	1:B:430:ARG:HD3	1.66	0.77
1:F:7:LYS:HZ1	1:F:100:ALA:N	1.81	0.77
1:B:7:LYS:NZ	1:B:101:TRP:HE3	1.81	0.77
1:E:120:LYS:H	1:E:120:LYS:CE	1.96	0.76
1:E:79:ASN:HB3	1:E:82:SER:OG	1.85	0.76
1:E:33:ARG:HH11	1:E:33:ARG:HG3	1.50	0.76
1:C:3:LYS:HD2	1:C:115:GLN:OE1	1.84	0.76
1:C:214:VAL:H	1:C:269:ASN:HD22	1.34	0.76
1:A:7:LYS:NZ	1:A:101:TRP:HE3	1.81	0.76
1:H:307:VAL:N	1:H:308:LYS:HE3	2.01	0.76
1:F:218:ALA:HA	1:F:241:THR:OG1	1.85	0.76
1:D:7:LYS:HZ1	1:D:100:ALA:N	1.83	0.76
1:F:119:PHE:HB3	1:F:120:LYS:HE2	1.67	0.76
1:G:33:ARG:HA	1:G:33:ARG:NE	2.01	0.76
1:E:7:LYS:HZ3	1:E:101:TRP:HE3	1.30	0.76
1:G:275:THR:HG22	1:G:277:CYS:N	2.02	0.75
1:H:308:LYS:H	1:H:308:LYS:CE	2.00	0.75
1:E:379:PRO:O	1:E:383:HIS:HE1	1.70	0.75
1:A:408:LEU:HD13	1:B:243:ILE:HG21	1.69	0.75
1:E:342:ARG:HG2	1:E:342:ARG:HH11	1.50	0.75
1:H:131:GLY:HA3	1:H:300:HIS:NE2	2.01	0.75
1:H:156:THR:O	1:H:160:VAL:HG23	1.86	0.75
1:H:120:LYS:CE	1:H:120:LYS:H	2.00	0.75
1:C:21:LEU:HD12	1:C:57:VAL:HG13	1.69	0.75
1:C:326:ARG:HD2	1:C:336:ILE:HG12	1.69	0.74
1:H:214:VAL:H	1:H:269:ASN:HD22	1.34	0.74
1:H:7:LYS:NZ	1:H:101:TRP:CE3	2.49	0.74
1:A:36:GLU:HB3	1:G:409:THR:HG22	1.68	0.74
1:F:223:VAL:HG12	1:F:274:THR:HB	1.70	0.74
1:G:221:GLY:O	1:G:225:LYS:HG3	1.86	0.74
1:E:343:LEU:HG	2:E:5432:NAD:N7N	2.01	0.74
1:E:374:HIS:CG	1:E:377:LYS:HE3	2.22	0.74
1:H:194:CYS:SG	1:H:223:VAL:HG13	2.27	0.74
1:A:7:LYS:HZ1	1:A:100:ALA:N	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:VAL:CG1	1:F:303:VAL:HB	2.19	0.73
1:B:353:PRO:CB	1:D:209:MET:HB2	2.18	0.73
1:H:101:TRP:HZ2	1:H:108:GLU:OE1	1.71	0.73
1:G:214:VAL:H	1:G:269:ASN:ND2	1.85	0.73
1:E:143:PRO:O	1:E:146:LEU:HB2	1.88	0.73
1:F:326:ARG:NH1	1:F:326:ARG:HG2	2.01	0.73
1:F:218:ALA:HB3	1:F:273:THR:HA	1.69	0.73
1:F:3:LYS:HD2	1:F:115:GLN:OE1	1.89	0.73
1:B:21:LEU:HD12	1:B:57:VAL:HG13	1.70	0.73
1:D:214:VAL:H	1:D:269:ASN:HD22	1.37	0.72
1:C:33:ARG:NH2	1:C:36:GLU:HB2	2.02	0.72
1:E:180:ASN:HA	1:E:185:LYS:HE3	1.71	0.72
1:A:7:LYS:HE2	1:A:112:CYS:SG	2.30	0.72
1:E:412:GLN:HG2	1:F:277:CYS:SG	2.30	0.72
1:G:3:LYS:HD3	1:G:115:GLN:HE22	1.54	0.72
1:C:10:ASP:HB3	1:C:13:LEU:HD22	1.71	0.72
1:F:80:ILE:HD11	1:F:342:ARG:HE	1.53	0.72
1:H:105:THR:OG1	1:H:108:GLU:HG3	1.88	0.71
1:G:7:LYS:HE3	1:G:99:PHE:HB3	1.71	0.71
1:F:37:MET:HG3	1:F:38:TYR:CE2	2.24	0.71
1:G:238:VAL:HB	1:G:256:TYR:CE1	2.25	0.71
1:E:120:LYS:N	1:E:120:LYS:HE2	2.05	0.71
1:A:209:MET:HB2	1:C:353:PRO:CB	2.21	0.71
1:E:33:ARG:HH21	1:E:36:GLU:HB2	1.54	0.71
1:D:326:ARG:HD2	1:D:336:ILE:HG12	1.71	0.71
1:A:21:LEU:HD12	1:A:57:VAL:HG13	1.72	0.71
1:C:33:ARG:HG3	1:C:33:ARG:HH11	1.56	0.71
1:C:275:THR:HG22	1:C:277:CYS:N	2.06	0.71
1:E:101:TRP:CH2	1:E:108:GLU:HB3	2.25	0.71
1:B:278:VAL:HG12	1:B:303:VAL:HB	1.72	0.71
1:H:56:THR:HG22	1:H:84:GLN:OE1	1.90	0.71
1:H:138:ILE:HD12	1:H:149:ILE:HD11	1.72	0.71
1:H:307:VAL:H	1:H:308:LYS:HE3	1.55	0.71
1:A:33:ARG:HH11	1:A:33:ARG:HG3	1.55	0.71
1:H:156:THR:HG23	1:H:159:GLY:H	1.56	0.71
1:B:129:ASP:OD2	1:B:135:THR:HG23	1.91	0.71
1:H:232:ARG:HH11	1:H:232:ARG:HG3	1.55	0.71
1:G:391:GLU:OE2	1:G:423:PRO:HA	1.90	0.71
1:F:7:LYS:HE2	1:F:112:CYS:SG	2.30	0.70
1:B:2:ASP:HB2	1:B:74:ARG:HH12	1.54	0.70
1:A:2:ASP:HB2	1:A:74:ARG:HH12	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:425:LYS:HE3	2:H:8432:NAD:H3B	1.72	0.70
1:G:33:ARG:NH2	1:G:36:GLU:HB2	2.03	0.70
1:B:2:ASP:HB3	1:B:3:LYS:HE3	1.72	0.70
1:F:3:LYS:HB2	1:F:4:LEU:HD12	1.74	0.70
1:E:7:LYS:HE3	1:E:99:PHE:HA	1.73	0.70
1:H:153:SER:HB3	1:H:364:GLN:HE22	1.55	0.70
1:A:169:ASN:HB2	1:A:171:ILE:HG12	1.73	0.70
1:D:10:ASP:HB3	1:D:13:LEU:HD22	1.73	0.70
1:G:275:THR:HG22	1:G:276:GLY:H	1.54	0.70
1:G:214:VAL:H	1:G:269:ASN:HD22	1.38	0.70
1:G:7:LYS:HE2	1:G:112:CYS:SG	2.32	0.70
1:F:167:MET:CE	1:F:380:VAL:HG12	2.22	0.70
1:G:138:ILE:HA	1:G:142:HIS:HB2	1.73	0.70
1:E:81:PHE:CE2	1:E:342:ARG:HG3	2.27	0.69
1:G:10:ASP:HB3	1:G:13:LEU:HD22	1.73	0.69
1:F:419:PRO:HB2	1:F:422:GLY:H	1.58	0.69
1:A:278:VAL:HG12	1:A:303:VAL:HB	1.73	0.69
1:A:198:LEU:HD22	1:A:227:CYS:SG	2.32	0.69
1:F:275:THR:HG22	1:F:277:CYS:N	2.07	0.69
1:G:127:ILE:HD11	1:G:149:ILE:HD13	1.74	0.69
1:D:150:ARG:HD3	1:D:375:PRO:HB3	1.75	0.69
1:A:210:ILE:HG22	1:A:236:ALA:HB2	1.74	0.69
1:D:308:LYS:CD	1:D:308:LYS:H	2.02	0.69
1:F:154:GLU:HB2	1:F:163:LEU:HD11	1.75	0.69
1:C:275:THR:HG22	1:C:276:GLY:N	2.07	0.69
1:B:143:PRO:O	1:B:146:LEU:HB2	1.93	0.69
1:G:142:HIS:HB3	1:G:145:LEU:HG	1.74	0.69
1:B:29:PRO:O	1:B:33:ARG:HB2	1.93	0.69
1:H:171:ILE:O	1:H:173:LYS:HG2	1.93	0.69
1:H:33:ARG:NH1	1:H:37:MET:SD	2.66	0.68
1:G:275:THR:HG21	1:G:277:CYS:HB3	1.75	0.68
1:H:232:ARG:NH1	1:H:232:ARG:HG3	2.08	0.68
1:B:326:ARG:HD2	1:B:336:ILE:HG12	1.74	0.68
1:A:2:ASP:OD2	1:A:118:HIS:HB2	1.94	0.68
1:G:310:LEU:HD22	1:G:327:TYR:CG	2.28	0.68
1:E:53:LEU:HD12	1:E:130:ASP:HB2	1.74	0.68
1:H:53:LEU:HG	1:H:130:ASP:HB2	1.74	0.68
1:D:29:PRO:O	1:D:33:ARG:HB2	1.93	0.68
1:G:33:ARG:NH1	1:G:37:MET:SD	2.67	0.68
1:F:105:THR:H	1:F:108:GLU:HB2	1.58	0.68
1:H:185:LYS:HD3	1:H:360:SER:OG	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:LEU:HB3	1:H:86:HIS:HA	1.73	0.68
1:E:362:THR:HG22	1:E:393:VAL:HG22	1.75	0.68
1:F:57:VAL:H	1:F:84:GLN:HE22	1.37	0.68
1:A:419:PRO:HB2	1:A:422:GLY:H	1.58	0.68
1:G:240:ILE:O	1:G:258:VAL:HA	1.92	0.68
1:E:13:LEU:HB3	1:E:86:HIS:HA	1.76	0.68
1:E:430:ARG:HA	1:F:430:ARG:HD3	1.74	0.68
1:E:7:LYS:HE3	1:E:99:PHE:CA	2.24	0.68
1:E:322:PRO:O	1:E:324:VAL:HG23	1.92	0.68
1:C:278:VAL:HG12	1:C:303:VAL:HB	1.73	0.68
1:A:3:LYS:HD2	1:A:115:GLN:OE1	1.92	0.68
1:E:2:ASP:HB3	1:E:3:LYS:HD2	1.75	0.68
1:F:353:PRO:HB2	1:H:209:MET:HB2	1.76	0.68
1:D:223:VAL:HG12	1:D:274:THR:HB	1.76	0.68
1:E:377:LYS:HD2	1:E:378:TYR:CE1	2.29	0.68
1:C:57:VAL:HG23	1:C:84:GLN:HE21	1.58	0.68
1:D:3:LYS:HD2	1:D:115:GLN:OE1	1.94	0.68
1:H:308:LYS:HE3	1:H:308:LYS:H	1.58	0.68
1:G:2:ASP:OD2	1:G:118:HIS:HB2	1.94	0.68
1:C:101:TRP:CH2	1:C:108:GLU:HB3	2.30	0.67
1:H:275:THR:HG22	1:H:276:GLY:N	2.08	0.67
1:G:105:THR:H	1:G:108:GLU:HB2	1.57	0.67
1:B:57:VAL:H	1:B:84:GLN:NE2	1.91	0.67
1:D:169:ASN:HB2	1:D:171:ILE:HG12	1.76	0.67
1:G:58:GLU:HG2	1:G:354:SER:HA	1.75	0.67
1:A:33:ARG:NH2	1:A:36:GLU:HB2	2.07	0.67
1:A:150:ARG:HD3	1:A:375:PRO:HB3	1.76	0.67
1:C:246:ILE:O	1:C:250:GLN:HG3	1.94	0.67
1:E:159:GLY:O	1:E:162:ASN:ND2	2.28	0.67
1:H:48:ARG:HD2	1:H:119:PHE:CB	2.24	0.67
1:C:210:ILE:HG22	1:C:236:ALA:HB2	1.75	0.67
1:E:3:LYS:H	1:E:3:LYS:HD2	1.59	0.67
1:E:300:HIS:HA	1:E:343:LEU:HD11	1.76	0.67
1:H:185:LYS:HD2	1:H:185:LYS:C	2.15	0.67
1:A:243:ILE:HG21	1:B:408:LEU:HD13	1.75	0.67
1:F:120:LYS:HE2	1:F:120:LYS:H	1.57	0.67
1:C:57:VAL:H	1:C:84:GLN:NE2	1.91	0.67
1:C:391:GLU:OE2	1:C:423:PRO:HA	1.94	0.67
1:D:410:GLU:O	1:D:414:GLN:HG2	1.95	0.67
1:D:57:VAL:HG23	1:D:84:GLN:HE21	1.59	0.67
1:C:7:LYS:HZ1	1:C:100:ALA:N	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:MET:HB2	1:D:353:PRO:HB2	1.77	0.66
1:C:419:PRO:HB2	1:C:422:GLY:H	1.58	0.66
1:E:408:LEU:HD13	1:F:243:ILE:HG21	1.76	0.66
1:E:195:ARG:NH1	1:E:229:GLN:NE2	2.35	0.66
1:E:81:PHE:CD2	1:E:342:ARG:HG3	2.30	0.66
1:C:4:LEU:HD13	1:C:99:PHE:HE1	1.60	0.66
1:E:275:THR:HG22	1:E:277:CYS:N	2.10	0.66
1:F:429:TYR:CE2	1:F:431:TYR:HA	2.30	0.66
1:E:7:LYS:O	1:E:7:LYS:NZ	2.25	0.66
1:H:7:LYS:HE3	1:H:99:PHE:CA	2.25	0.66
1:E:101:TRP:HH2	1:E:108:GLU:HB3	1.60	0.66
1:H:183:VAL:O	1:H:187:LYS:HB2	1.94	0.66
1:E:243:ILE:HG21	1:F:408:LEU:HD13	1.77	0.66
1:C:240:ILE:O	1:C:258:VAL:HA	1.96	0.66
1:F:199:ILE:HD11	1:F:231:LEU:HD23	1.78	0.66
1:D:275:THR:HG22	1:D:276:GLY:N	2.10	0.66
1:H:300:HIS:H	2:H:8432:NAD:H1D	1.59	0.66
1:A:308:LYS:CD	1:A:308:LYS:H	2.08	0.66
1:D:120:LYS:H	1:D:120:LYS:CE	2.06	0.66
1:H:74:ARG:HG3	1:H:119:PHE:CZ	2.31	0.66
1:D:129:ASP:OD2	1:D:135:THR:HG23	1.94	0.66
1:H:267:GLU:HA	1:H:290:LYS:HE3	1.77	0.66
1:C:2:ASP:HB2	1:C:74:ARG:HH12	1.61	0.66
1:H:342:ARG:HH11	1:H:342:ARG:HG2	1.60	0.66
1:E:408:LEU:CD1	1:F:243:ILE:HG21	2.26	0.66
1:D:48:ARG:HD2	1:D:119:PHE:CB	2.26	0.65
1:H:139:HIS:HA	1:H:146:LEU:HD11	1.78	0.65
1:F:136:ASN:O	1:F:140:THR:HG23	1.96	0.65
1:B:7:LYS:HZ1	1:B:100:ALA:CA	2.08	0.65
1:E:38:TYR:HB2	1:E:69:LEU:HD11	1.77	0.65
1:D:275:THR:HG22	1:D:277:CYS:N	2.11	0.65
1:G:58:GLU:CG	1:G:354:SER:HA	2.26	0.65
1:D:419:PRO:HB2	1:D:422:GLY:H	1.62	0.65
1:A:29:PRO:O	1:A:33:ARG:HB2	1.96	0.65
1:F:155:GLU:HG3	1:F:364:GLN:OE1	1.97	0.65
1:G:21:LEU:O	1:G:25:GLU:HG3	1.97	0.65
1:B:169:ASN:HB2	1:B:171:ILE:HG12	1.78	0.65
1:E:224:GLY:HA2	1:E:274:THR:HG21	1.78	0.65
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.61	0.65
1:F:310:LEU:HD13	1:F:327:TYR:CD1	2.31	0.65
1:E:315:VAL:HB	1:E:328:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ASP:OD2	1:G:135:THR:HG23	1.96	0.65
1:C:48:ARG:HD2	1:C:119:PHE:HB2	1.78	0.65
1:F:78:CYS:HA	1:F:109:TYR:OH	1.97	0.65
1:D:33:ARG:HH11	1:D:33:ARG:HG3	1.61	0.65
1:D:278:VAL:HG12	1:D:303:VAL:HB	1.79	0.65
1:F:379:PRO:O	1:F:383:HIS:HE1	1.80	0.65
1:E:210:ILE:HG22	1:E:236:ALA:HB2	1.79	0.65
1:H:138:ILE:HG22	1:H:146:LEU:HD12	1.78	0.64
1:G:169:ASN:HB2	1:G:171:ILE:HG12	1.78	0.64
1:D:4:LEU:N	1:D:4:LEU:HD12	2.12	0.64
1:E:105:THR:OG1	1:E:108:GLU:HG3	1.97	0.64
1:B:419:PRO:HB2	1:B:422:GLY:H	1.60	0.64
1:B:33:ARG:NH1	1:B:33:ARG:HG3	2.04	0.64
1:C:48:ARG:HD2	1:C:119:PHE:CB	2.28	0.64
1:G:153:SER:HB2	1:G:368:GLN:NE2	2.12	0.64
1:B:2:ASP:CB	1:B:3:LYS:HE3	2.27	0.64
1:C:2:ASP:OD2	1:C:118:HIS:HB2	1.98	0.64
1:E:374:HIS:ND1	1:E:377:LYS:HE3	2.13	0.64
1:B:2:ASP:OD2	1:B:118:HIS:HB2	1.97	0.64
1:H:224:GLY:HA2	1:H:274:THR:HG21	1.80	0.64
1:C:146:LEU:HA	1:C:149:ILE:HD12	1.80	0.64
1:C:243:ILE:HG21	1:D:408:LEU:HD13	1.79	0.64
1:F:146:LEU:HA	1:F:149:ILE:HD12	1.79	0.64
1:B:4:LEU:HD13	1:B:99:PHE:HE1	1.62	0.64
1:E:345:ASN:O	1:E:349:ALA:HB3	1.97	0.64
1:B:26:ASN:O	1:B:400:LYS:HE2	1.96	0.64
1:E:121:ASP:N	1:E:121:ASP:OD1	2.28	0.64
1:A:53:LEU:CD1	1:A:130:ASP:HB2	2.27	0.64
1:E:308:LYS:O	1:E:312:GLU:HG3	1.98	0.64
1:F:297:ASN:OD1	1:F:304:GLU:HG3	1.98	0.64
1:G:33:ARG:NH2	1:G:37:MET:HG2	2.13	0.64
1:C:7:LYS:HE2	1:C:112:CYS:SG	2.38	0.64
1:G:238:VAL:HB	1:G:256:TYR:HE1	1.63	0.64
1:D:283:GLY:HA3	1:D:309:TRP:CE2	2.33	0.64
1:H:167:MET:HG2	1:H:172:LEU:HB3	1.80	0.64
1:H:188:PHE:O	1:H:192:TYR:HB2	1.97	0.63
1:A:416:LEU:HD21	1:B:277:CYS:HB2	1.79	0.63
1:H:419:PRO:HB2	1:H:422:GLY:N	2.10	0.63
1:H:29:PRO:O	1:H:33:ARG:HB2	1.99	0.63
1:D:2:ASP:HB2	1:D:74:ARG:NH1	2.13	0.63
1:E:21:LEU:HD12	1:E:57:VAL:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:HD2	1:B:119:PHE:CB	2.27	0.63
1:E:171:ILE:O	1:E:173:LYS:HG2	1.98	0.63
1:E:209:MET:SD	1:G:356:VAL:HB	2.38	0.63
1:F:172:LEU:HD22	1:F:174:VAL:H	1.63	0.63
1:G:91:ILE:HG23	1:G:96:ILE:HB	1.80	0.63
1:A:4:LEU:HD13	1:A:99:PHE:HE1	1.64	0.63
1:H:120:LYS:HE2	1:H:120:LYS:N	2.05	0.63
1:E:275:THR:HG21	1:E:280:ILE:HD11	1.81	0.63
1:F:4:LEU:CD2	1:F:7:LYS:HB3	2.28	0.63
1:H:7:LYS:HG2	1:H:111:TRP:CH2	2.34	0.63
1:A:150:ARG:HD2	1:A:372:TRP:HA	1.81	0.63
1:F:342:ARG:HG2	1:F:342:ARG:HH11	1.62	0.63
1:A:7:LYS:HZ1	1:A:100:ALA:CA	2.12	0.63
1:B:7:LYS:NZ	1:B:100:ALA:N	2.46	0.63
1:A:101:TRP:CH2	1:A:108:GLU:HB3	2.34	0.63
1:G:105:THR:OG1	1:G:108:GLU:HG3	1.98	0.63
1:F:198:LEU:CD2	1:F:227:CYS:HB3	2.29	0.63
1:B:210:ILE:HG22	1:B:236:ALA:HB2	1.81	0.63
1:G:178:ASN:OD1	1:G:181:ASP:HB2	1.98	0.63
1:C:33:ARG:HG3	1:C:33:ARG:NH1	2.13	0.62
1:D:48:ARG:HD2	1:D:119:PHE:HB2	1.80	0.62
1:F:430:ARG:HG3	1:F:430:ARG:HH11	1.64	0.62
1:F:292:ASP:OD1	1:F:326:ARG:NE	2.29	0.62
1:E:307:VAL:H	1:E:308:LYS:HE3	1.64	0.62
1:H:136:ASN:O	1:H:140:THR:HG23	1.98	0.62
1:E:425:LYS:HD2	1:E:429:TYR:CD2	2.34	0.62
1:A:7:LYS:HE3	1:A:99:PHE:HB3	1.80	0.62
1:H:48:ARG:HD2	1:H:119:PHE:HB2	1.80	0.62
1:H:162:ASN:O	1:H:166:MET:HG3	1.98	0.62
1:H:57:VAL:O	1:H:61:VAL:HG23	2.00	0.62
1:A:48:ARG:HD2	1:A:119:PHE:CB	2.29	0.62
1:A:7:LYS:HE3	1:A:99:PHE:CA	2.30	0.62
1:D:101:TRP:CH2	1:D:108:GLU:HB3	2.34	0.62
1:E:48:ARG:HD2	1:E:119:PHE:HB2	1.82	0.62
1:A:391:GLU:OE2	1:A:423:PRO:HA	1.99	0.62
1:F:119:PHE:HB2	1:F:122:GLY:O	1.99	0.62
1:E:373:THR:HG22	1:E:374:HIS:CD2	2.34	0.62
1:C:26:ASN:O	1:C:400:LYS:HE2	1.99	0.62
1:A:214:VAL:H	1:A:269:ASN:HD22	1.47	0.62
1:B:167:MET:HE1	1:B:380:VAL:O	1.99	0.62
1:H:33:ARG:NH2	1:H:37:MET:HG2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:ILE:HG22	1:G:203:LYS:HG3	1.82	0.62
1:G:295:VAL:HG12	1:G:337:LEU:HD23	1.82	0.62
1:H:141:LYS:HB3	1:H:142:HIS:ND1	2.15	0.62
1:E:212:GLY:O	1:G:401:LEU:HD22	1.98	0.62
1:F:3:LYS:HD3	1:F:115:GLN:HE22	1.64	0.62
1:A:48:ARG:HD2	1:A:119:PHE:HB2	1.82	0.62
1:H:239:ILE:HG23	1:H:257:GLU:HG2	1.82	0.62
1:D:240:ILE:O	1:D:258:VAL:HA	1.98	0.62
1:F:388:LYS:HG2	1:F:423:PRO:HG3	1.81	0.62
1:B:33:ARG:NH2	1:B:36:GLU:HB2	2.11	0.62
1:D:4:LEU:HD13	1:D:99:PHE:HE1	1.63	0.62
1:H:4:LEU:HD12	1:H:4:LEU:N	2.14	0.62
1:B:167:MET:HE3	1:B:381:GLY:HA2	1.82	0.62
1:A:129:ASP:OD2	1:A:135:THR:HG23	1.99	0.62
1:B:246:ILE:O	1:B:250:GLN:HG3	2.00	0.62
1:B:240:ILE:O	1:B:258:VAL:HA	1.99	0.62
1:E:81:PHE:O	1:E:102:LYS:HE3	2.00	0.62
1:A:33:ARG:NE	1:A:33:ARG:HA	2.14	0.62
1:D:2:ASP:OD2	1:D:118:HIS:HB2	2.00	0.62
1:H:86:HIS:ND1	1:H:87:ALA:N	2.48	0.62
1:C:129:ASP:OD2	1:C:135:THR:HG23	1.99	0.62
1:E:23:ILE:HD11	1:G:320:ILE:HG13	1.81	0.62
1:E:74:ARG:HB3	1:E:116:THR:HB	1.81	0.61
1:F:275:THR:HG22	1:F:276:GLY:N	2.15	0.61
1:G:4:LEU:HD13	1:G:99:PHE:CE1	2.35	0.61
1:C:29:PRO:O	1:C:33:ARG:HB2	2.00	0.61
1:B:101:TRP:CH2	1:B:108:GLU:HB3	2.34	0.61
1:H:275:THR:CG2	1:H:277:CYS:HB2	2.30	0.61
1:C:388:LYS:HG2	1:C:423:PRO:HD3	1.81	0.61
1:A:119:PHE:HB2	1:A:122:GLY:O	2.00	0.61
1:F:259:THR:HG22	1:F:260:THR:H	1.66	0.61
1:H:240:ILE:O	1:H:258:VAL:HA	1.99	0.61
1:F:377:LYS:O	1:F:377:LYS:HG2	2.00	0.61
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.65	0.61
1:A:7:LYS:NZ	1:A:100:ALA:N	2.49	0.61
1:F:105:THR:HG23	1:F:108:GLU:OE1	2.01	0.61
1:A:275:THR:HG22	1:A:276:GLY:N	2.15	0.61
1:A:13:LEU:HB3	1:A:86:HIS:HA	1.82	0.61
1:D:120:LYS:HE2	1:D:120:LYS:N	2.09	0.61
1:E:247:ASN:ND2	1:F:425:LYS:HE2	2.15	0.61
1:F:143:PRO:O	1:F:146:LEU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:LYS:HZ1	1:H:250:GLN:HE22	1.48	0.61
1:F:7:LYS:O	1:F:7:LYS:NZ	2.33	0.61
1:A:154:GLU:HG3	1:A:160:VAL:HG23	1.81	0.61
1:F:249:LEU:O	1:F:253:MET:HG2	2.00	0.61
1:H:33:ARG:NH2	1:H:37:MET:N	2.33	0.61
1:B:3:LYS:H	1:B:3:LYS:HE3	1.65	0.61
1:F:79:ASN:HB3	1:F:82:SER:OG	2.00	0.61
1:G:307:VAL:HG22	1:G:337:LEU:HD11	1.83	0.61
1:H:308:LYS:CD	1:H:308:LYS:H	2.13	0.61
1:B:7:LYS:HE3	1:B:99:PHE:HB3	1.81	0.61
1:A:57:VAL:H	1:A:84:GLN:NE2	1.98	0.61
1:A:188:PHE:O	1:A:192:TYR:HB2	2.00	0.61
1:H:395:GLU:HA	1:H:398:LEU:HD22	1.83	0.60
1:D:7:LYS:HZ1	1:D:100:ALA:CA	2.13	0.60
1:D:246:ILE:O	1:D:250:GLN:HG3	2.01	0.60
1:E:353:PRO:CB	1:G:209:MET:HB2	2.30	0.60
1:B:308:LYS:CD	1:B:308:LYS:H	2.13	0.60
1:E:206:THR:HG23	1:E:338:LEU:HD21	1.82	0.60
1:B:33:ARG:NE	1:B:33:ARG:HA	2.16	0.60
1:D:377:LYS:HD2	1:D:378:TYR:CE1	2.35	0.60
1:C:7:LYS:HZ1	1:C:100:ALA:CA	2.14	0.60
1:E:246:ILE:HD11	1:F:390:ASP:HB3	1.84	0.60
1:A:240:ILE:O	1:A:258:VAL:HA	2.01	0.60
1:H:178:ASN:ND2	1:H:181:ASP:HB2	2.16	0.60
1:B:7:LYS:HE2	1:B:112:CYS:SG	2.41	0.60
1:D:7:LYS:HG2	1:D:111:TRP:CZ3	2.37	0.60
1:C:250:GLN:O	1:C:254:GLU:HG2	2.02	0.60
1:C:232:ARG:HH11	1:C:232:ARG:HG3	1.66	0.60
1:B:33:ARG:NH1	1:B:37:MET:SD	2.74	0.60
1:B:275:THR:HG22	1:B:277:CYS:N	2.07	0.60
1:C:4:LEU:HD12	1:C:4:LEU:N	2.15	0.60
1:G:138:ILE:HG23	1:G:142:HIS:HB2	1.84	0.60
1:H:249:LEU:O	1:H:253:MET:HG2	2.00	0.60
1:B:48:ARG:HD2	1:B:119:PHE:HB2	1.83	0.60
1:G:162:ASN:HA	1:G:165:LYS:HB2	1.84	0.60
1:F:113:ILE:O	1:F:116:THR:HG23	2.02	0.60
1:G:4:LEU:HD13	1:G:99:PHE:HE1	1.67	0.60
1:A:275:THR:HG22	1:A:277:CYS:N	2.12	0.60
1:B:146:LEU:HA	1:B:149:ILE:HD12	1.84	0.60
1:C:143:PRO:O	1:C:146:LEU:HB2	2.01	0.60
1:B:119:PHE:HB2	1:B:122:GLY:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ARG:HB3	1:E:119:PHE:CD2	2.36	0.60
1:D:7:LYS:HE3	1:D:99:PHE:HB3	1.83	0.60
1:F:44:LEU:HB3	1:F:71:ALA:HB2	1.84	0.60
1:E:152:ILE:HB	1:E:176:ALA:CB	2.32	0.60
1:C:13:LEU:HB3	1:C:86:HIS:HA	1.84	0.60
1:A:57:VAL:HG23	1:A:84:GLN:HE21	1.67	0.60
1:D:150:ARG:HD2	1:D:372:TRP:HA	1.84	0.60
1:G:127:ILE:HG23	1:G:134:LEU:HD13	1.84	0.59
1:H:79:ASN:HB3	1:H:82:SER:OG	2.01	0.59
1:B:154:GLU:HG3	1:B:160:VAL:HG23	1.84	0.59
1:D:308:LYS:HD2	1:D:308:LYS:H	1.66	0.59
1:H:167:MET:SD	1:H:381:GLY:HA2	2.42	0.59
1:B:179:VAL:HG13	1:B:363:ASN:HB3	1.85	0.59
1:A:223:VAL:HG12	1:A:274:THR:HB	1.83	0.59
1:E:419:PRO:HB2	1:E:422:GLY:HA3	1.83	0.59
1:C:223:VAL:HG12	1:C:274:THR:HB	1.83	0.59
1:G:198:LEU:HD22	1:G:227:CYS:SG	2.42	0.59
1:D:56:THR:HA	1:D:84:GLN:HB2	1.85	0.59
1:E:308:LYS:H	1:E:308:LYS:CE	2.13	0.59
1:G:419:PRO:HB2	1:G:422:GLY:H	1.67	0.59
1:G:275:THR:CG2	1:G:276:GLY:N	2.66	0.59
1:G:7:LYS:NZ	1:G:101:TRP:CE3	2.54	0.59
1:A:209:MET:O	1:A:213:LYS:HD2	2.01	0.59
1:G:307:VAL:HG21	1:G:340:GLU:O	2.03	0.59
1:H:225:LYS:HZ2	1:H:250:GLN:HE22	1.49	0.59
1:H:19:LYS:O	1:H:23:ILE:HG13	2.03	0.59
1:H:429:TYR:CE2	1:H:431:TYR:HA	2.37	0.59
1:C:343:LEU:HG	2:C:3432:NAD:N7N	2.17	0.59
1:D:57:VAL:HG23	1:D:84:GLN:NE2	2.18	0.59
1:D:146:LEU:HA	1:D:149:ILE:HD12	1.84	0.59
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.18	0.59
1:G:151:GLY:HA2	1:G:174:VAL:HG23	1.83	0.59
1:C:169:ASN:HB2	1:C:171:ILE:HG12	1.85	0.59
1:F:183:VAL:HG21	1:F:431:TYR:CE1	2.38	0.59
1:D:53:LEU:CD1	1:D:130:ASP:HB2	2.31	0.59
1:G:35:ARG:HE	1:G:65:THR:HA	1.66	0.59
1:G:190:ASN:HB3	1:G:223:VAL:HG23	1.83	0.59
1:B:111:TRP:O	1:B:115:GLN:HG2	2.02	0.59
1:A:179:VAL:HG13	1:A:363:ASN:HB3	1.84	0.59
1:G:54:HIS:HA	1:G:77:SER:OG	2.02	0.59
1:B:2:ASP:HB2	1:B:74:ARG:NH1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:LYS:HG2	1:F:269:ASN:HB3	1.85	0.59
1:H:387:LYS:HZ3	1:H:431:TYR:HE1	1.51	0.59
1:B:57:VAL:HG23	1:B:84:GLN:HE21	1.68	0.59
1:A:300:HIS:H	2:A:1432:NAD:H1D	1.68	0.59
1:D:232:ARG:HH11	1:D:232:ARG:HG3	1.66	0.59
1:H:33:ARG:NH2	1:H:36:GLU:HB2	2.18	0.58
1:D:33:ARG:NE	1:D:33:ARG:HA	2.17	0.58
1:D:119:PHE:HB2	1:D:122:GLY:O	2.03	0.58
1:B:275:THR:HG22	1:B:276:GLY:N	2.16	0.58
1:F:419:PRO:HB2	1:F:422:GLY:N	2.17	0.58
1:A:307:VAL:H	1:A:308:LYS:HE3	1.68	0.58
1:D:138:ILE:HG22	1:D:146:LEU:HD13	1.85	0.58
1:E:178:ASN:HB2	1:E:382:VAL:CG2	2.34	0.58
1:D:210:ILE:HG22	1:D:236:ALA:HB2	1.84	0.58
1:A:283:GLY:HA3	1:A:309:TRP:CE2	2.38	0.58
1:C:7:LYS:HE3	1:C:99:PHE:HB3	1.84	0.58
1:F:4:LEU:HD13	1:F:99:PHE:CE1	2.26	0.58
1:H:365:VAL:O	1:H:369:ILE:HG13	2.02	0.58
1:H:278:VAL:HG12	1:H:303:VAL:CB	2.30	0.58
1:G:387:LYS:HG2	1:G:423:PRO:HB3	1.84	0.58
1:F:273:THR:HG22	1:F:280:ILE:HG21	1.85	0.58
1:C:56:THR:HA	1:C:84:GLN:HB2	1.84	0.58
1:F:167:MET:HE1	1:F:380:VAL:HG12	1.82	0.58
1:A:127:ILE:HG23	1:A:134:LEU:HD13	1.84	0.58
1:A:138:ILE:HG22	1:A:146:LEU:HD13	1.85	0.58
1:D:2:ASP:CB	1:D:74:ARG:HH12	2.15	0.58
1:F:57:VAL:O	1:F:60:ALA:HB3	2.04	0.58
1:F:4:LEU:N	1:F:4:LEU:CD1	2.65	0.58
1:F:425:LYS:HD2	1:F:429:TYR:CE2	2.38	0.58
1:G:395:GLU:CA	1:G:398:LEU:HD13	2.31	0.58
1:D:307:VAL:H	1:D:308:LYS:HE3	1.66	0.58
1:C:198:LEU:HD22	1:C:227:CYS:SG	2.44	0.58
1:D:154:GLU:HG3	1:D:160:VAL:HG23	1.85	0.58
1:B:120:LYS:CE	1:B:120:LYS:H	2.14	0.58
1:G:7:LYS:HE3	1:G:99:PHE:CB	2.34	0.58
1:B:150:ARG:HD2	1:B:372:TRP:HA	1.85	0.58
1:A:353:PRO:CB	1:C:209:MET:HB2	2.32	0.58
1:A:167:MET:HE3	1:A:381:GLY:HA2	1.85	0.58
1:H:33:ARG:O	1:H:37:MET:HG2	2.03	0.58
1:D:33:ARG:HG3	1:D:33:ARG:NH1	2.18	0.58
1:A:408:LEU:CD1	1:B:243:ILE:HG21	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:LEU:HD21	1:H:361:PHE:HB3	1.86	0.58
1:C:33:ARG:HA	1:C:33:ARG:NE	2.19	0.58
1:F:59:THR:O	1:F:62:LEU:HB3	2.04	0.58
1:G:300:HIS:H	2:G:7432:NAD:H1D	1.68	0.58
1:A:33:ARG:NH1	1:A:37:MET:SD	2.76	0.58
1:H:275:THR:HG22	1:H:277:CYS:N	2.18	0.58
1:D:138:ILE:HG22	1:D:146:LEU:CD1	2.33	0.58
1:A:49:ILE:HD12	1:A:71:ALA:HB1	1.86	0.58
1:E:4:LEU:HD11	1:E:111:TRP:CZ2	2.39	0.58
1:E:44:LEU:HD12	1:E:69:LEU:HB3	1.86	0.58
1:E:206:THR:CG2	1:E:338:LEU:HD21	2.34	0.58
1:E:178:ASN:ND2	1:E:384:PHE:HE1	2.02	0.58
1:A:410:GLU:O	1:A:414:GLN:HG2	2.03	0.58
1:C:63:ILE:O	1:C:67:VAL:HG23	2.04	0.58
1:C:377:LYS:HD2	1:C:378:TYR:CE1	2.39	0.58
1:G:7:LYS:HE3	1:G:99:PHE:CA	2.34	0.58
1:H:275:THR:HG21	1:H:277:CYS:HB2	1.86	0.58
1:H:141:LYS:HB3	1:H:142:HIS:CE1	2.38	0.58
1:C:388:LYS:HG2	1:C:423:PRO:HG3	1.85	0.58
1:B:343:LEU:HG	2:B:2432:NAD:N7N	2.19	0.58
1:H:261:MET:HA	1:H:264:ALA:HB3	1.85	0.58
1:E:184:THR:HA	1:E:188:PHE:CE1	2.39	0.58
1:A:33:ARG:HG3	1:A:33:ARG:NH1	2.17	0.57
1:G:387:LYS:O	1:G:391:GLU:HG3	2.04	0.57
1:A:143:PRO:O	1:A:146:LEU:HB2	2.04	0.57
1:C:232:ARG:NH1	1:C:232:ARG:HG3	2.19	0.57
1:G:277:CYS:SG	1:H:412:GLN:HB3	2.44	0.57
1:A:388:LYS:HG2	1:A:423:PRO:HG3	1.85	0.57
1:F:125:ASN:ND2	1:F:372:TRP:CH2	2.72	0.57
1:G:365:VAL:O	1:G:369:ILE:HG13	2.05	0.57
1:G:182:SER:HB2	1:G:185:LYS:HB2	1.87	0.57
1:D:26:ASN:O	1:D:400:LYS:HE2	2.04	0.57
1:C:41:SER:HB2	1:C:43:PRO:HD3	1.84	0.57
1:F:4:LEU:HD21	1:F:111:TRP:HH2	1.69	0.57
1:G:143:PRO:O	1:G:146:LEU:HB2	2.05	0.57
1:G:171:ILE:O	1:G:173:LYS:HE3	2.05	0.57
1:G:419:PRO:HB2	1:G:422:GLY:HA3	1.85	0.57
1:F:362:THR:CG2	1:F:393:VAL:HG22	2.33	0.57
1:A:252:ALA:O	1:D:212:GLY:HA2	2.04	0.57
1:B:410:GLU:O	1:B:414:GLN:HG2	2.05	0.57
1:F:42:LYS:NZ	1:F:68:ALA:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLY:HA2	1:C:252:ALA:O	2.04	0.57
1:A:246:ILE:O	1:A:250:GLN:HG3	2.04	0.57
1:E:143:PRO:HA	1:E:146:LEU:HD22	1.87	0.57
1:B:209:MET:O	1:B:213:LYS:HD2	2.04	0.57
1:D:127:ILE:HD11	1:D:138:ILE:HD12	1.87	0.57
1:D:143:PRO:O	1:D:146:LEU:HB2	2.03	0.57
1:A:146:LEU:HA	1:A:149:ILE:HD12	1.86	0.57
1:G:185:LYS:HD3	1:G:360:SER:OG	2.05	0.57
1:D:111:TRP:O	1:D:115:GLN:HG2	2.04	0.57
1:C:57:VAL:O	1:C:60:ALA:HB3	2.04	0.57
1:C:57:VAL:HG23	1:C:84:GLN:NE2	2.19	0.57
1:C:307:VAL:H	1:C:308:LYS:HE3	1.70	0.57
1:C:154:GLU:HG3	1:C:160:VAL:HG23	1.87	0.57
1:B:7:LYS:HG2	1:B:111:TRP:CZ3	2.40	0.57
1:B:178:ASN:ND2	1:B:181:ASP:HB2	2.20	0.57
1:H:91:ILE:HG23	1:H:96:ILE:HB	1.85	0.57
1:G:245:PRO:HA	1:H:398:LEU:HD21	1.86	0.57
1:F:57:VAL:HG22	1:F:87:ALA:HB2	1.86	0.57
1:H:127:ILE:HD11	1:H:149:ILE:HD13	1.87	0.57
1:F:283:GLY:HA2	1:F:286:PHE:HB2	1.86	0.57
1:F:129:ASP:OD2	1:F:135:THR:HG23	2.05	0.57
1:G:44:LEU:HB3	1:G:71:ALA:HB2	1.86	0.57
1:C:101:TRP:HH2	1:C:108:GLU:HB3	1.68	0.57
1:E:29:PRO:O	1:E:33:ARG:HB2	2.05	0.57
1:G:310:LEU:HD13	1:G:327:TYR:CE1	2.40	0.57
1:C:127:ILE:HG23	1:C:134:LEU:HD13	1.86	0.57
1:E:201:GLY:HA2	1:E:349:ALA:HB2	1.86	0.57
1:F:344:VAL:O	1:F:348:CYS:HB2	2.04	0.57
1:B:377:LYS:HD2	1:B:378:TYR:CE1	2.39	0.57
1:G:397:HIS:ND1	1:G:397:HIS:N	2.53	0.57
1:E:209:MET:HB2	1:G:353:PRO:CB	2.31	0.57
1:H:246:ILE:O	1:H:250:GLN:HG3	2.05	0.57
1:G:75:TRP:HH2	1:G:128:LEU:HD13	1.70	0.57
1:B:358:SER:HB3	1:B:397:HIS:NE2	2.19	0.57
1:E:292:ASP:CG	1:E:326:ARG:HH21	2.08	0.57
1:E:259:THR:HG22	1:E:260:THR:H	1.70	0.57
1:E:142:HIS:N	1:E:143:PRO:HD3	2.19	0.56
1:E:243:ILE:HG21	1:F:408:LEU:CD1	2.34	0.56
1:E:56:THR:HG22	1:E:84:GLN:OE1	2.05	0.56
1:G:194:CYS:SG	1:G:223:VAL:HG22	2.45	0.56
1:E:261:MET:O	1:E:265:CYS:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:PHE:HA	1:H:192:TYR:CD2	2.40	0.56
1:F:199:ILE:HG22	1:F:203:LYS:HG3	1.87	0.56
1:B:13:LEU:HB3	1:B:86:HIS:HA	1.87	0.56
1:C:53:LEU:CD1	1:C:130:ASP:HB2	2.34	0.56
1:G:91:ILE:HD12	1:G:96:ILE:HD12	1.88	0.56
1:C:300:HIS:H	2:C:3432:NAD:H1D	1.70	0.56
1:F:246:ILE:O	1:F:250:GLN:HG3	2.05	0.56
1:A:406:THR:HB	1:B:242:GLU:O	2.05	0.56
1:G:263:GLU:HA	1:G:266:LYS:HE2	1.87	0.56
1:C:410:GLU:O	1:C:414:GLN:HG2	2.05	0.56
1:G:7:LYS:O	1:G:7:LYS:NZ	2.30	0.56
1:A:250:GLN:O	1:A:254:GLU:HG2	2.05	0.56
1:D:41:SER:HB2	1:D:43:PRO:HD3	1.86	0.56
1:B:153:SER:HB3	1:B:364:GLN:HE22	1.70	0.56
1:A:2:ASP:HB2	1:A:74:ARG:NH1	2.20	0.56
1:A:171:ILE:O	1:A:173:LYS:HG2	2.06	0.56
1:E:279:ASP:HA	1:E:282:LEU:HD11	1.87	0.56
1:E:75:TRP:HH2	1:E:128:LEU:HD13	1.70	0.56
1:A:33:ARG:O	1:A:37:MET:HG2	2.05	0.56
1:A:4:LEU:N	1:A:4:LEU:HD12	2.20	0.56
1:H:343:LEU:HG	2:H:8432:NAD:N7N	2.21	0.56
1:G:142:HIS:N	1:G:143:PRO:HD3	2.20	0.56
1:C:358:SER:HB3	1:C:397:HIS:NE2	2.21	0.56
1:D:63:ILE:O	1:D:67:VAL:HG23	2.06	0.56
1:F:35:ARG:HE	1:F:65:THR:HA	1.70	0.56
1:D:300:HIS:H	2:D:4432:NAD:H1D	1.70	0.56
1:D:209:MET:O	1:D:213:LYS:HD2	2.05	0.56
1:C:7:LYS:HG2	1:C:111:TRP:CZ3	2.40	0.56
1:C:150:ARG:HD2	1:C:372:TRP:HA	1.88	0.56
1:E:6:TYR:HA	1:E:99:PHE:CE1	2.41	0.56
1:A:225:LYS:NZ	1:A:250:GLN:HE22	2.03	0.56
1:F:297:ASN:CG	1:F:304:GLU:HG3	2.26	0.56
1:B:225:LYS:NZ	1:B:250:GLN:HE22	2.04	0.56
1:B:44:LEU:HB3	1:B:71:ALA:HB2	1.87	0.56
1:H:44:LEU:HD13	1:H:71:ALA:HB2	1.88	0.56
1:G:31:LEU:HD21	1:G:361:PHE:HB3	1.88	0.56
1:H:74:ARG:HG3	1:H:119:PHE:CE2	2.41	0.56
1:E:17:GLY:O	1:E:21:LEU:HD13	2.05	0.56
1:B:334:ARG:O	1:B:335:ILE:HD13	2.06	0.56
1:E:297:ASN:OD1	1:E:304:GLU:HG3	2.05	0.56
1:G:33:ARG:HG3	1:G:33:ARG:NH1	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:MET:O	1:E:213:LYS:HD2	2.05	0.56
1:F:425:LYS:HD2	1:F:429:TYR:CD2	2.41	0.56
1:E:419:PRO:HB2	1:E:422:GLY:H	1.71	0.56
1:H:334:ARG:O	1:H:335:ILE:HD13	2.06	0.56
1:B:391:GLU:OE2	1:B:423:PRO:HA	2.06	0.56
1:D:48:ARG:HD2	1:D:119:PHE:CG	2.41	0.56
1:A:326:ARG:HD2	1:A:336:ILE:CG1	2.35	0.56
1:E:362:THR:CG2	1:E:393:VAL:HG22	2.35	0.56
1:F:101:TRP:HZ2	1:F:108:GLU:OE2	1.90	0.55
1:H:225:LYS:NZ	1:H:250:GLN:NE2	2.54	0.55
1:E:300:HIS:H	2:E:5432:NAD:H1D	1.71	0.55
1:B:56:THR:HA	1:B:84:GLN:HB2	1.87	0.55
1:G:185:LYS:O	1:G:189:ASP:HB3	2.05	0.55
1:E:297:ASN:O	1:E:344:VAL:HB	2.06	0.55
1:E:409:THR:H	1:E:412:GLN:HE21	1.54	0.55
1:A:430:ARG:HG3	1:A:430:ARG:HH11	1.71	0.55
1:A:278:VAL:HA	1:A:303:VAL:O	2.05	0.55
1:C:283:GLY:HA3	1:C:309:TRP:CE2	2.41	0.55
1:G:259:THR:HA	1:H:404:LYS:HB2	1.87	0.55
1:H:33:ARG:CZ	1:H:33:ARG:O	2.54	0.55
1:G:250:GLN:HG2	1:H:188:PHE:CZ	2.40	0.55
1:C:7:LYS:NZ	1:C:100:ALA:N	2.53	0.55
1:D:7:LYS:NZ	1:D:100:ALA:N	2.54	0.55
1:H:244:ASP:CB	1:H:247:ASN:HD22	2.15	0.55
1:G:167:MET:HG2	1:G:172:LEU:HD12	1.87	0.55
1:C:142:HIS:N	1:C:143:PRO:HD3	2.22	0.55
1:D:232:ARG:NH1	1:D:232:ARG:HG3	2.19	0.55
1:E:175:PRO:HD3	1:E:380:VAL:HG22	1.87	0.55
1:G:278:VAL:HG12	1:G:303:VAL:HB	1.87	0.55
1:C:153:SER:HB3	1:C:364:GLN:HE22	1.70	0.55
1:F:206:THR:HG22	1:F:338:LEU:HD21	1.89	0.55
1:B:47:ALA:HA	1:B:125:ASN:HD21	1.71	0.55
1:G:3:LYS:HB2	1:G:4:LEU:HD12	1.88	0.55
1:F:199:ILE:CD1	1:F:231:LEU:HD23	2.36	0.55
1:B:171:ILE:O	1:B:173:LYS:HG2	2.06	0.55
1:B:232:ARG:HG3	1:B:232:ARG:NH1	2.19	0.55
1:C:167:MET:HG2	1:C:172:LEU:HD12	1.89	0.55
1:B:136:ASN:O	1:B:140:THR:HG23	2.06	0.55
1:H:407:LYS:NZ	1:H:420:ILE:HD13	2.21	0.55
1:D:7:LYS:HE3	1:D:99:PHE:CA	2.36	0.55
1:A:419:PRO:HB2	1:A:422:GLY:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:GLU:OE1	1:H:209:MET:HG3	2.06	0.55
1:D:136:ASN:O	1:D:140:THR:HG23	2.06	0.55
1:D:430:ARG:HH11	1:D:430:ARG:HG3	1.72	0.55
1:C:308:LYS:CD	1:C:308:LYS:H	2.18	0.55
1:G:49:ILE:HD12	1:G:71:ALA:HB1	1.88	0.55
1:E:75:TRP:CH2	1:E:128:LEU:HD13	2.41	0.55
1:G:33:ARG:HH22	1:G:37:MET:CG	2.20	0.55
1:A:2:ASP:CB	1:A:3:LYS:HE3	2.37	0.55
1:E:141:LYS:C	1:E:143:PRO:HD3	2.27	0.55
1:E:321:LYS:HB2	1:E:322:PRO:HD2	1.87	0.55
1:E:178:ASN:HB2	1:E:382:VAL:HG23	1.89	0.55
1:H:362:THR:HG22	1:H:393:VAL:HG22	1.89	0.55
1:B:356:VAL:HB	1:D:209:MET:SD	2.46	0.55
1:E:278:VAL:HG13	1:F:415:TYR:CZ	2.42	0.55
1:G:308:LYS:H	1:G:308:LYS:CD	2.20	0.55
1:E:13:LEU:CB	1:E:86:HIS:HA	2.36	0.55
1:D:343:LEU:HG	2:D:4432:NAD:N7N	2.21	0.55
1:D:391:GLU:OE2	1:D:423:PRO:HA	2.07	0.55
1:B:223:VAL:HG12	1:B:274:THR:HB	1.89	0.55
1:G:150:ARG:O	1:G:150:ARG:HG3	2.06	0.55
1:G:3:LYS:CD	1:G:115:GLN:HE22	2.19	0.55
1:E:33:ARG:NE	1:E:33:ARG:CA	2.69	0.55
1:C:155:GLU:O	1:C:180:ASN:HB2	2.07	0.55
1:H:180:ASN:HA	1:H:185:LYS:HE3	1.89	0.55
1:A:21:LEU:O	1:A:25:GLU:HG3	2.06	0.55
1:D:13:LEU:HB3	1:D:86:HIS:HA	1.89	0.55
1:A:44:LEU:HB3	1:A:71:ALA:HB2	1.88	0.55
1:G:180:ASN:HA	1:G:185:LYS:HE3	1.88	0.55
1:E:124:LEU:HD21	1:E:149:ILE:HD11	1.89	0.55
1:D:101:TRP:HH2	1:D:108:GLU:HB3	1.70	0.54
1:G:99:PHE:N	1:G:99:PHE:CD2	2.75	0.54
1:C:124:LEU:HD11	1:C:138:ILE:HD11	1.89	0.54
1:G:413:ALA:HB2	1:G:420:ILE:HG12	1.89	0.54
1:B:214:VAL:H	1:B:269:ASN:HD22	1.53	0.54
1:G:101:TRP:CZ2	1:G:104:GLU:HB3	2.42	0.54
1:E:7:LYS:NZ	1:E:101:TRP:CE3	2.67	0.54
1:B:387:LYS:HE2	1:B:431:TYR:OH	2.07	0.54
1:G:311:ASN:OD1	1:G:327:TYR:HE2	1.90	0.54
1:F:353:PRO:CB	1:H:209:MET:HB2	2.36	0.54
1:D:142:HIS:N	1:D:143:PRO:HD3	2.22	0.54
1:H:167:MET:HG2	1:H:172:LEU:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:ILE:HG22	1:F:236:ALA:HB2	1.90	0.54
1:E:211:ALA:HB2	1:E:234:PHE:O	2.07	0.54
1:F:7:LYS:HG2	1:F:111:TRP:CH2	2.42	0.54
1:E:208:VAL:HG22	1:E:209:MET:N	2.22	0.54
1:E:105:THR:HG23	1:E:108:GLU:OE1	2.07	0.54
1:B:53:LEU:CD1	1:B:130:ASP:HB2	2.35	0.54
1:E:343:LEU:HG	2:E:5432:NAD:H72N	1.72	0.54
1:H:33:ARG:NH2	1:H:36:GLU:CB	2.71	0.54
1:C:111:TRP:O	1:C:115:GLN:HG2	2.07	0.54
1:F:57:VAL:N	1:F:84:GLN:NE2	2.46	0.54
1:G:7:LYS:HZ1	1:G:100:ALA:N	2.06	0.54
1:E:196:GLU:HG2	1:G:234:PHE:CD1	2.42	0.54
1:E:77:SER:O	1:E:109:TYR:HE1	1.91	0.54
1:H:271:PHE:HB2	1:H:295:VAL:HG13	1.90	0.54
1:E:407:LYS:HE2	1:E:420:ILE:HG21	1.90	0.54
1:B:188:PHE:O	1:B:192:TYR:HB2	2.08	0.54
1:A:205:ALA:HB1	1:A:338:LEU:HD22	1.88	0.54
1:C:57:VAL:H	1:C:84:GLN:HE22	1.55	0.54
1:H:142:HIS:ND1	1:H:142:HIS:N	2.56	0.54
1:F:317:LYS:HD2	1:F:327:TYR:CE2	2.42	0.54
1:A:212:GLY:HA2	1:D:252:ALA:O	2.08	0.54
1:A:358:SER:HB3	1:A:397:HIS:NE2	2.22	0.54
1:C:7:LYS:NZ	1:C:101:TRP:CE3	2.67	0.54
1:D:21:LEU:O	1:D:25:GLU:HG3	2.07	0.54
1:H:225:LYS:HZ2	1:H:250:GLN:NE2	2.05	0.54
1:B:172:LEU:HD22	1:B:174:VAL:H	1.71	0.54
1:E:152:ILE:HD11	1:E:174:VAL:HG13	1.90	0.54
1:C:172:LEU:HD22	1:C:174:VAL:H	1.73	0.54
1:E:3:LYS:HD2	1:E:3:LYS:N	2.21	0.54
1:B:155:GLU:O	1:B:180:ASN:HB2	2.08	0.54
1:C:430:ARG:HG3	1:C:430:ARG:HH11	1.73	0.54
1:G:101:TRP:HZ2	1:G:108:GLU:CD	2.10	0.54
1:E:379:PRO:O	1:E:383:HIS:CE1	2.57	0.54
1:H:129:ASP:OD2	1:H:135:THR:HG23	2.07	0.54
1:A:279:ASP:HA	1:A:282:LEU:HD11	1.89	0.54
1:H:185:LYS:O	1:H:189:ASP:HB3	2.08	0.54
1:B:419:PRO:HB2	1:B:422:GLY:N	2.23	0.54
1:G:345:ASN:O	1:G:349:ALA:HB3	2.07	0.54
1:E:126:MET:HE3	1:E:372:TRP:HB2	1.89	0.54
1:E:161:HIS:CD2	1:E:165:LYS:HD3	2.43	0.54
1:H:29:PRO:HD2	1:H:397:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:THR:CG2	1:F:276:GLY:N	2.71	0.54
1:C:419:PRO:HB2	1:C:422:GLY:N	2.22	0.54
1:D:49:ILE:HD12	1:D:71:ALA:HB1	1.88	0.54
1:B:24:ALA:O	1:B:28:MET:HG3	2.08	0.54
1:C:2:ASP:HB2	1:C:74:ARG:NH1	2.23	0.54
1:H:4:LEU:HD11	1:H:111:TRP:HZ2	1.73	0.54
1:H:7:LYS:HE3	1:H:99:PHE:C	2.27	0.54
1:F:198:LEU:HD21	1:F:231:LEU:HD21	1.89	0.54
1:G:306:ASP:OD1	1:G:308:LYS:HD2	2.08	0.54
1:F:310:LEU:HD13	1:F:327:TYR:CE1	2.43	0.54
1:B:49:ILE:HD12	1:B:71:ALA:HB1	1.90	0.54
1:F:328:LEU:HD12	1:F:329:LEU:N	2.22	0.54
1:G:95:GLY:O	1:G:97:PRO:HD3	2.08	0.54
1:G:158:THR:HB	2:G:7432:NAD:O3D	2.08	0.53
1:H:142:HIS:N	1:H:143:PRO:HD3	2.23	0.53
1:E:425:LYS:HD2	1:E:429:TYR:CG	2.44	0.53
1:H:198:LEU:HD22	1:H:227:CYS:CB	2.36	0.53
1:C:47:ALA:HA	1:C:125:ASN:HD21	1.73	0.53
1:E:142:HIS:HB3	1:E:145:LEU:HD12	1.90	0.53
1:F:364:GLN:O	1:F:368:GLN:HG2	2.07	0.53
1:C:127:ILE:HD11	1:C:138:ILE:HD12	1.90	0.53
1:A:258:VAL:HB	1:B:403:VAL:HG13	1.90	0.53
1:D:199:ILE:HG22	1:D:203:LYS:HG3	1.90	0.53
1:G:184:THR:HA	1:G:188:PHE:CD1	2.43	0.53
1:C:188:PHE:O	1:C:192:TYR:HB2	2.07	0.53
1:E:275:THR:HG22	1:E:276:GLY:N	2.24	0.53
1:D:57:VAL:H	1:D:84:GLN:NE2	2.05	0.53
1:E:386:PRO:HG2	1:E:389:LEU:HG	1.89	0.53
1:D:47:ALA:HA	1:D:125:ASN:HD21	1.73	0.53
1:G:92:ALA:HB2	1:G:98:VAL:CG1	2.39	0.53
1:C:7:LYS:HE3	1:C:99:PHE:CA	2.38	0.53
1:A:55:MET:HB3	1:A:83:THR:CG2	2.33	0.53
1:F:342:ARG:HG2	1:F:342:ARG:NH1	2.22	0.53
1:F:142:HIS:N	1:F:143:PRO:HD3	2.23	0.53
1:E:183:VAL:HG11	1:E:431:TYR:CG	2.43	0.53
1:D:44:LEU:HB2	1:D:69:LEU:O	2.07	0.53
1:G:275:THR:CG2	1:G:276:GLY:H	2.20	0.53
1:F:118:HIS:HA	1:F:123:PRO:HA	1.90	0.53
1:E:250:GLN:HG2	1:F:188:PHE:CZ	2.44	0.53
1:F:227:CYS:O	1:F:231:LEU:HG	2.08	0.53
1:B:127:ILE:HD11	1:B:138:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LYS:H	1:C:120:LYS:CE	2.14	0.53
1:E:44:LEU:HB3	1:E:71:ALA:HB2	1.90	0.53
1:A:388:LYS:HG2	1:A:423:PRO:HD3	1.90	0.53
1:A:343:LEU:HG	2:A:1432:NAD:N7N	2.23	0.53
1:E:184:THR:HA	1:E:188:PHE:CD1	2.44	0.53
1:E:177:ILE:HG13	1:E:371:LEU:HD21	1.91	0.53
1:E:129:ASP:OD2	1:E:135:THR:HG22	2.07	0.53
1:E:48:ARG:HD2	1:E:119:PHE:CB	2.39	0.53
1:B:300:HIS:H	2:B:2432:NAD:H1D	1.74	0.53
1:B:198:LEU:HD22	1:B:227:CYS:SG	2.48	0.53
1:C:247:ASN:HD21	1:D:425:LYS:HE2	1.72	0.53
1:A:194:CYS:SG	1:A:223:VAL:HG22	2.49	0.53
1:F:320:ILE:HG13	1:H:23:ILE:HD11	1.91	0.53
1:C:247:ASN:ND2	1:D:425:LYS:HE2	2.24	0.53
1:H:27:GLU:O	1:H:355:PHE:HA	2.08	0.53
1:F:101:TRP:HZ2	1:F:108:GLU:CD	2.11	0.53
1:F:120:LYS:CE	1:F:120:LYS:H	2.21	0.53
1:E:33:ARG:HG3	1:E:33:ARG:NH1	2.22	0.53
1:G:252:ALA:HB2	1:H:403:VAL:HG21	1.91	0.53
1:D:142:HIS:N	1:D:143:PRO:CD	2.72	0.53
1:G:150:ARG:HD3	1:G:375:PRO:HB3	1.91	0.53
1:E:401:LEU:HD22	1:G:212:GLY:O	2.08	0.53
1:H:156:THR:CG2	1:H:159:GLY:H	2.21	0.52
1:H:179:VAL:HG11	1:H:364:GLN:HG2	1.91	0.52
1:E:119:PHE:HB2	1:E:122:GLY:O	2.08	0.52
1:F:300:HIS:HA	1:F:343:LEU:HD11	1.91	0.52
1:B:283:GLY:HA3	1:B:309:TRP:CE2	2.44	0.52
1:E:28:MET:HG2	1:E:354:SER:O	2.08	0.52
1:B:4:LEU:HD12	1:B:4:LEU:N	2.24	0.52
1:E:315:VAL:HG23	1:E:330:LYS:CG	2.31	0.52
1:G:183:VAL:HG22	1:H:430:ARG:CZ	2.40	0.52
1:D:388:LYS:HG2	1:D:423:PRO:HG3	1.90	0.52
1:B:252:ALA:O	1:C:212:GLY:HA2	2.09	0.52
1:F:54:HIS:HB3	1:F:82:SER:CB	2.37	0.52
1:D:275:THR:HG22	1:D:276:GLY:H	1.74	0.52
1:E:343:LEU:HD23	1:E:346:LEU:CD1	2.39	0.52
1:G:59:THR:O	1:G:62:LEU:HB3	2.09	0.52
1:F:257:GLU:HG3	1:G:237:ARG:NH2	2.25	0.52
1:A:259:THR:HA	1:B:404:LYS:HB2	1.91	0.52
1:G:7:LYS:HD3	1:G:111:TRP:HZ3	1.73	0.52
1:F:387:LYS:HE2	1:F:431:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:PHE:HB2	1:C:122:GLY:O	2.09	0.52
1:F:175:PRO:HB3	1:F:379:PRO:O	2.10	0.52
1:E:356:VAL:O	1:E:359:ASN:HB2	2.09	0.52
1:G:154:GLU:HG3	1:G:160:VAL:HG23	1.92	0.52
1:H:35:ARG:O	1:H:39:SER:HB2	2.10	0.52
1:G:29:PRO:O	1:G:33:ARG:HB2	2.09	0.52
1:B:138:ILE:HG22	1:B:146:LEU:HD13	1.90	0.52
1:E:21:LEU:O	1:E:25:GLU:HG3	2.09	0.52
1:A:403:VAL:HG13	1:B:258:VAL:HB	1.92	0.52
1:H:407:LYS:HZ3	1:H:420:ILE:HD13	1.75	0.52
1:F:316:GLU:HB3	1:F:328:LEU:HB3	1.91	0.52
1:D:179:VAL:HG13	1:D:363:ASN:HB3	1.91	0.52
1:A:345:ASN:O	1:A:349:ALA:HB3	2.09	0.52
1:F:114:GLU:HA	1:F:117:LEU:HG	1.91	0.52
1:F:33:ARG:O	1:F:37:MET:HG2	2.10	0.52
1:F:17:GLY:HA2	1:F:86:HIS:CD2	2.45	0.52
1:C:275:THR:CG2	1:C:276:GLY:N	2.72	0.52
1:A:35:ARG:O	1:A:39:SER:HB2	2.09	0.52
1:A:7:LYS:HG2	1:A:111:TRP:CZ3	2.44	0.52
1:G:210:ILE:HG22	1:G:236:ALA:HB2	1.91	0.52
1:H:131:GLY:CA	1:H:300:HIS:NE2	2.72	0.52
1:E:428:HIS:NE2	1:F:181:ASP:OD2	2.42	0.52
1:B:279:ASP:HA	1:B:282:LEU:HD11	1.91	0.52
1:H:2:ASP:CA	1:H:3:LYS:HE3	2.40	0.52
1:G:7:LYS:HD3	1:G:111:TRP:CZ3	2.45	0.52
1:A:155:GLU:O	1:A:180:ASN:HB2	2.10	0.52
1:E:153:SER:CB	1:E:364:GLN:HE22	2.18	0.52
1:H:141:LYS:C	1:H:143:PRO:HD3	2.29	0.52
1:G:134:LEU:HD22	1:G:138:ILE:HD11	1.92	0.52
1:A:307:VAL:N	1:A:308:LYS:HE3	2.25	0.52
1:G:116:THR:O	1:G:119:PHE:HE1	1.92	0.52
1:F:7:LYS:HE3	1:F:99:PHE:HA	1.92	0.52
1:E:101:TRP:HZ2	1:E:108:GLU:OE1	1.92	0.52
1:G:35:ARG:NE	1:G:65:THR:HA	2.24	0.52
1:F:127:ILE:HD11	1:F:138:ILE:CD1	2.40	0.52
1:A:142:HIS:HB3	1:A:145:LEU:HG	1.92	0.52
1:G:75:TRP:CH2	1:G:128:LEU:HD13	2.45	0.52
1:G:286:PHE:C	1:G:288:GLN:H	2.13	0.52
1:E:297:ASN:HB2	1:E:305:ILE:HD12	1.91	0.52
1:C:409:THR:H	1:C:412:GLN:HE21	1.58	0.52
1:D:127:ILE:HG23	1:D:134:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ASN:O	1:D:349:ALA:HB3	2.09	0.52
1:D:188:PHE:O	1:D:192:TYR:HB2	2.10	0.52
1:E:266:LYS:HD3	1:E:288:GLN:HG2	1.92	0.52
1:F:33:ARG:NH1	1:F:37:MET:SD	2.77	0.51
1:F:7:LYS:HE3	1:F:99:PHE:CA	2.41	0.51
1:F:209:MET:SD	1:H:356:VAL:HB	2.50	0.51
1:H:73:VAL:HG12	1:H:74:ARG:N	2.25	0.51
1:D:283:GLY:HA2	1:D:286:PHE:HB2	1.92	0.51
1:B:250:GLN:O	1:B:254:GLU:HG2	2.10	0.51
1:G:179:VAL:HG13	1:G:363:ASN:HB3	1.91	0.51
1:B:41:SER:HB2	1:B:43:PRO:HD3	1.91	0.51
1:E:343:LEU:HD23	1:E:346:LEU:HD12	1.92	0.51
1:F:297:ASN:HB2	1:F:305:ILE:HD12	1.92	0.51
1:C:179:VAL:HG13	1:C:363:ASN:HB3	1.92	0.51
1:G:33:ARG:HH21	1:G:36:GLU:CB	2.09	0.51
1:A:7:LYS:HE3	1:A:99:PHE:CB	2.41	0.51
1:G:308:LYS:H	1:G:308:LYS:HE3	1.75	0.51
1:A:48:ARG:HD2	1:A:119:PHE:CG	2.45	0.51
1:E:2:ASP:OD2	1:E:118:HIS:HB2	2.10	0.51
1:G:203:LYS:O	1:G:207:ASP:N	2.44	0.51
1:C:138:ILE:HG22	1:C:146:LEU:HD13	1.91	0.51
1:F:141:LYS:HB3	1:F:142:HIS:ND1	2.26	0.51
1:F:322:PRO:O	1:F:323:GLN:HB2	2.10	0.51
1:F:19:LYS:O	1:F:22:ASP:HB2	2.09	0.51
1:G:275:THR:CG2	1:G:277:CYS:HB3	2.40	0.51
1:C:275:THR:HG22	1:C:276:GLY:H	1.75	0.51
1:F:3:LYS:C	1:F:4:LEU:HD12	2.30	0.51
1:F:198:LEU:HG	1:F:199:ILE:N	2.25	0.51
1:G:307:VAL:O	1:G:310:LEU:HB2	2.09	0.51
1:H:360:SER:O	1:H:363:ASN:HB2	2.09	0.51
1:B:409:THR:H	1:B:412:GLN:HE21	1.58	0.51
1:A:4:LEU:HD11	1:A:111:TRP:CZ2	2.46	0.51
1:C:209:MET:O	1:C:213:LYS:HD2	2.11	0.51
1:C:124:LEU:HD11	1:C:138:ILE:CD1	2.40	0.51
1:C:138:ILE:HG22	1:C:146:LEU:CD1	2.40	0.51
1:G:159:GLY:O	1:G:162:ASN:ND2	2.42	0.51
1:A:300:HIS:HA	1:A:343:LEU:HD11	1.92	0.51
1:H:326:ARG:HD2	1:H:336:ILE:HG12	1.92	0.51
1:F:389:LEU:O	1:F:392:ALA:HB3	2.11	0.51
1:H:29:PRO:O	1:H:33:ARG:N	2.43	0.51
1:B:429:TYR:CE2	1:B:431:TYR:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HA	1:A:84:GLN:HB2	1.92	0.51
1:E:308:LYS:CD	1:E:308:LYS:H	2.24	0.51
1:C:171:ILE:O	1:C:173:LYS:HG2	2.11	0.51
1:D:167:MET:HE3	1:D:381:GLY:HA2	1.93	0.51
1:A:41:SER:HB2	1:A:43:PRO:HD3	1.91	0.51
1:C:33:ARG:O	1:C:37:MET:HG2	2.10	0.51
1:B:57:VAL:O	1:B:60:ALA:HB3	2.10	0.51
1:H:369:ILE:O	1:H:373:THR:HB	2.11	0.51
1:H:362:THR:CG2	1:H:393:VAL:HG22	2.41	0.51
1:H:275:THR:CG2	1:H:276:GLY:N	2.73	0.51
1:H:155:GLU:O	1:H:180:ASN:HB2	2.10	0.51
1:F:138:ILE:HG22	1:F:146:LEU:HD13	1.93	0.51
1:E:152:ILE:HD12	1:E:176:ALA:HB2	1.93	0.51
1:A:167:MET:HG2	1:A:172:LEU:HD12	1.93	0.51
1:D:162:ASN:O	1:D:166:MET:HG3	2.10	0.51
1:H:7:LYS:HG2	1:H:111:TRP:CZ3	2.45	0.51
1:C:244:ASP:HB3	1:C:247:ASN:HB2	1.93	0.51
1:F:386:PRO:HD2	1:F:389:LEU:HD12	1.93	0.51
1:D:158:THR:O	1:D:161:HIS:HB3	2.11	0.51
1:C:2:ASP:CB	1:C:3:LYS:HE3	2.41	0.50
1:C:185:LYS:C	1:C:185:LYS:HD2	2.31	0.50
1:B:142:HIS:N	1:B:143:PRO:HD3	2.26	0.50
1:E:53:LEU:CD1	1:E:130:ASP:HB2	2.41	0.50
1:G:152:ILE:HG13	1:G:174:VAL:CG2	2.41	0.50
1:E:188:PHE:HA	1:E:192:TYR:CD2	2.46	0.50
1:B:283:GLY:HA2	1:B:286:PHE:HB2	1.92	0.50
1:B:306:ASP:OD2	1:B:309:TRP:HB2	2.11	0.50
1:D:167:MET:HG2	1:D:172:LEU:HD12	1.93	0.50
1:H:7:LYS:HE3	1:H:99:PHE:HA	1.92	0.50
1:A:172:LEU:HD22	1:A:174:VAL:H	1.76	0.50
1:G:279:ASP:OD2	1:H:411:LYS:HD3	2.10	0.50
1:A:317:LYS:HD2	1:A:327:TYR:CZ	2.46	0.50
1:A:32:MET:O	1:A:36:GLU:HG3	2.10	0.50
1:B:33:ARG:O	1:B:37:MET:HG2	2.11	0.50
1:H:275:THR:HG22	1:H:277:CYS:H	1.74	0.50
1:E:319:ASN:ND2	1:E:321:LYS:O	2.45	0.50
1:A:142:HIS:N	1:A:143:PRO:HD3	2.26	0.50
1:F:152:ILE:HB	1:F:176:ALA:HB2	1.93	0.50
1:F:130:ASP:OD1	1:F:156:THR:HB	2.11	0.50
1:H:99:PHE:O	1:H:112:CYS:SG	2.69	0.50
1:H:7:LYS:NZ	1:H:100:ALA:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:ARG:HB3	1:H:119:PHE:CD2	2.46	0.50
1:G:152:ILE:HB	1:G:176:ALA:HB2	1.93	0.50
1:D:306:ASP:OD2	1:D:309:TRP:HB2	2.11	0.50
1:G:389:LEU:O	1:G:392:ALA:HB3	2.11	0.50
1:E:137:LEU:O	1:E:137:LEU:HD12	2.11	0.50
1:H:32:MET:O	1:H:36:GLU:HG3	2.12	0.50
1:F:7:LYS:HG2	1:F:111:TRP:CZ3	2.46	0.50
1:A:120:LYS:H	1:A:120:LYS:CE	2.16	0.50
1:D:307:VAL:N	1:D:308:LYS:HE3	2.27	0.50
1:C:225:LYS:HZ3	1:C:250:GLN:HE22	1.60	0.50
1:A:138:ILE:HG22	1:A:146:LEU:CD1	2.42	0.50
1:A:178:ASN:ND2	1:A:181:ASP:HB2	2.26	0.50
1:F:76:SER:HB3	1:F:116:THR:HG21	1.94	0.50
1:H:44:LEU:HB3	1:H:71:ALA:HB2	1.94	0.50
1:D:279:ASP:HA	1:D:282:LEU:HD11	1.92	0.50
1:G:41:SER:HB2	1:G:43:PRO:HD3	1.92	0.50
1:F:413:ALA:HB2	1:F:420:ILE:HG12	1.92	0.50
1:E:303:VAL:HG21	1:F:415:TYR:OH	2.10	0.50
1:H:3:LYS:HD2	1:H:3:LYS:H	1.75	0.50
1:H:342:ARG:NH1	1:H:342:ARG:HG2	2.24	0.50
1:G:53:LEU:HG	1:G:130:ASP:OD2	2.11	0.50
1:F:286:PHE:HA	1:F:289:MET:HG3	1.94	0.50
1:B:7:LYS:HE3	1:B:99:PHE:CA	2.42	0.50
1:A:208:VAL:CG2	1:A:213:LYS:HE2	2.42	0.50
1:A:430:ARG:NH1	1:A:430:ARG:HG3	2.27	0.50
1:H:343:LEU:HG	2:H:8432:NAD:H72N	1.77	0.50
1:H:114:GLU:OE2	1:H:142:HIS:NE2	2.45	0.50
1:B:127:ILE:HG23	1:B:134:LEU:HD13	1.93	0.50
1:G:142:HIS:HB3	1:G:145:LEU:CG	2.41	0.50
1:C:225:LYS:NZ	1:C:250:GLN:HE22	2.09	0.50
1:D:167:MET:HE1	1:D:380:VAL:O	2.11	0.50
1:A:63:ILE:O	1:A:67:VAL:HG23	2.12	0.50
1:H:386:PRO:HG2	1:H:389:LEU:CD1	2.29	0.50
1:G:33:ARG:HH22	1:G:37:MET:HG2	1.77	0.50
1:A:101:TRP:HZ2	1:A:108:GLU:OE1	1.94	0.50
1:B:120:LYS:N	1:B:120:LYS:HE2	2.17	0.50
1:E:37:MET:HG3	1:E:38:TYR:CD2	2.46	0.50
1:D:127:ILE:HG21	1:D:135:THR:HG22	1.94	0.50
1:C:127:ILE:HG21	1:C:135:THR:HG22	1.93	0.50
1:E:329:LEU:C	1:E:331:ASN:H	2.15	0.50
1:D:177:ILE:HD12	1:D:371:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TRP:HH2	1:B:108:GLU:HB3	1.76	0.50
1:H:250:GLN:O	1:H:254:GLU:HG2	2.11	0.50
1:H:18:ARG:HH22	1:H:64:GLU:CD	2.14	0.50
1:A:377:LYS:HD2	1:A:378:TYR:CE1	2.47	0.50
1:D:153:SER:HB3	1:D:364:GLN:HE22	1.76	0.50
1:G:404:LYS:HB2	1:H:259:THR:HA	1.94	0.50
1:H:4:LEU:HD12	1:H:4:LEU:H	1.75	0.49
1:D:430:ARG:NH1	1:D:430:ARG:HG3	2.27	0.49
1:E:419:PRO:HB2	1:E:422:GLY:CA	2.42	0.49
1:G:73:VAL:HG12	1:G:74:ARG:N	2.27	0.49
1:A:317:LYS:HD2	1:A:327:TYR:CE2	2.47	0.49
1:D:208:VAL:CG2	1:D:213:LYS:HE2	2.42	0.49
1:C:430:ARG:HG3	1:C:430:ARG:NH1	2.27	0.49
1:F:99:PHE:CD2	1:F:99:PHE:N	2.79	0.49
1:E:240:ILE:O	1:E:258:VAL:HA	2.13	0.49
1:F:183:VAL:HB	1:F:390:ASP:OD2	2.12	0.49
1:C:412:GLN:HG2	1:D:277:CYS:SG	2.52	0.49
1:F:66:LEU:O	1:F:71:ALA:HB3	2.12	0.49
1:G:419:PRO:HB2	1:G:422:GLY:N	2.27	0.49
1:B:184:THR:HA	1:B:188:PHE:CD1	2.47	0.49
1:G:48:ARG:HD2	1:G:119:PHE:CB	2.42	0.49
1:E:127:ILE:HD11	1:E:138:ILE:HD12	1.93	0.49
1:B:127:ILE:HG21	1:B:135:THR:HG22	1.94	0.49
1:D:142:HIS:O	1:D:145:LEU:HG	2.13	0.49
1:G:171:ILE:O	1:G:173:LYS:HG2	2.11	0.49
1:F:127:ILE:HD11	1:F:138:ILE:HD12	1.93	0.49
1:G:278:VAL:CG1	1:G:303:VAL:HB	2.42	0.49
1:G:279:ASP:HA	1:G:282:LEU:HD11	1.94	0.49
1:E:154:GLU:O	1:E:179:VAL:HB	2.12	0.49
1:A:153:SER:HB3	1:A:364:GLN:HE22	1.77	0.49
1:H:150:ARG:HD3	1:H:375:PRO:HB3	1.94	0.49
1:B:199:ILE:HG22	1:B:203:LYS:HG3	1.94	0.49
1:E:80:ILE:HG22	1:E:104:GLU:HB2	1.94	0.49
1:H:183:VAL:HG11	1:H:431:TYR:CG	2.47	0.49
1:D:224:GLY:HA2	1:D:274:THR:HG21	1.93	0.49
1:F:374:HIS:CG	1:F:377:LYS:HE3	2.48	0.49
1:H:35:ARG:NE	1:H:65:THR:OG1	2.45	0.49
1:B:2:ASP:CB	1:B:74:ARG:HH12	2.23	0.49
1:G:198:LEU:HD22	1:G:227:CYS:CB	2.43	0.49
1:G:386:PRO:HG2	1:G:389:LEU:HD12	1.93	0.49
1:C:79:ASN:HB3	1:C:82:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LYS:HD2	1:C:327:TYR:CZ	2.48	0.49
1:C:49:ILE:HD12	1:C:71:ALA:HB1	1.93	0.49
1:D:409:THR:H	1:D:412:GLN:HE21	1.61	0.49
1:B:79:ASN:HB3	1:B:82:SER:CB	2.43	0.49
1:G:7:LYS:HG2	1:G:111:TRP:CH2	2.48	0.49
1:F:49:ILE:HD13	1:F:368:GLN:OE1	2.13	0.49
1:C:48:ARG:HD2	1:C:119:PHE:CG	2.47	0.49
1:B:167:MET:HG2	1:B:172:LEU:HD12	1.95	0.49
1:G:419:PRO:HB2	1:G:422:GLY:CA	2.42	0.49
1:A:244:ASP:HB3	1:A:247:ASN:HB2	1.94	0.49
1:F:27:GLU:HB3	1:F:354:SER:OG	2.11	0.49
1:E:250:GLN:O	1:E:254:GLU:HG2	2.12	0.49
1:G:430:ARG:NH1	1:G:430:ARG:HG3	2.26	0.49
1:G:142:HIS:HB3	1:G:145:LEU:CD1	2.42	0.49
1:B:224:GLY:HA2	1:B:274:THR:HG21	1.95	0.49
1:D:206:THR:HG23	1:D:338:LEU:HD21	1.95	0.49
1:A:24:ALA:O	1:A:28:MET:HG3	2.13	0.49
1:A:79:ASN:HB3	1:A:82:SER:CB	2.42	0.49
1:D:6:TYR:OH	1:D:11:ILE:HD13	2.12	0.49
1:H:409:THR:OG1	1:H:412:GLN:HG3	2.12	0.49
1:D:225:LYS:NZ	1:D:250:GLN:HE22	2.11	0.49
1:C:430:ARG:CA	1:D:430:ARG:HD3	2.38	0.49
1:H:127:ILE:HG23	1:H:134:LEU:HD12	1.94	0.49
1:F:369:ILE:O	1:F:373:THR:HB	2.13	0.49
1:G:150:ARG:HD2	1:G:372:TRP:CE3	2.47	0.49
1:F:156:THR:HG22	1:F:159:GLY:H	1.77	0.49
1:E:5:PRO:O	1:E:97:PRO:HB3	2.13	0.49
1:H:358:SER:HB3	1:H:397:HIS:NE2	2.27	0.49
1:F:223:VAL:HG12	1:F:274:THR:CB	2.42	0.49
1:B:79:ASN:HB3	1:B:82:SER:OG	2.12	0.49
1:F:28:MET:CB	1:F:358:SER:HB2	2.43	0.49
1:B:205:ALA:HB1	1:B:338:LEU:HD22	1.94	0.49
1:H:206:THR:O	1:H:207:ASP:HB2	2.12	0.49
1:G:287:GLU:HG3	1:G:309:TRP:CZ2	2.48	0.49
1:E:246:ILE:O	1:E:250:GLN:HG3	2.13	0.48
1:E:319:ASN:HD21	1:E:321:LYS:C	2.16	0.48
1:F:379:PRO:O	1:F:383:HIS:CE1	2.64	0.48
1:D:300:HIS:HA	1:D:343:LEU:HD11	1.95	0.48
1:G:386:PRO:O	1:G:389:LEU:N	2.42	0.48
1:B:345:ASN:O	1:B:349:ALA:HB3	2.13	0.48
1:A:101:TRP:HH2	1:A:108:GLU:HB3	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:LYS:H	1:F:120:LYS:CD	2.25	0.48
1:F:430:ARG:HG3	1:F:430:ARG:NH1	2.28	0.48
1:D:419:PRO:HB2	1:D:422:GLY:N	2.25	0.48
1:D:79:ASN:HB3	1:D:82:SER:CB	2.43	0.48
1:H:128:LEU:HG	1:H:364:GLN:NE2	2.29	0.48
1:B:21:LEU:O	1:B:25:GLU:HG3	2.12	0.48
1:B:142:HIS:HB3	1:B:145:LEU:HG	1.94	0.48
1:F:142:HIS:N	1:F:143:PRO:CD	2.76	0.48
1:F:320:ILE:HD13	1:F:320:ILE:N	2.27	0.48
1:D:172:LEU:HD22	1:D:174:VAL:H	1.78	0.48
1:B:72:GLU:OE2	1:B:120:LYS:HE3	2.13	0.48
1:C:183:VAL:HG11	1:D:246:ILE:HG21	1.95	0.48
1:C:430:ARG:HD3	1:D:430:ARG:CA	2.33	0.48
1:E:101:TRP:HZ2	1:E:108:GLU:CD	2.17	0.48
1:C:79:ASN:HB3	1:C:82:SER:HB3	1.95	0.48
1:D:24:ALA:O	1:D:28:MET:HG3	2.14	0.48
1:H:409:THR:H	1:H:412:GLN:HE21	1.62	0.48
1:B:7:LYS:NZ	1:B:101:TRP:CE3	2.69	0.48
1:H:198:LEU:CD2	1:H:227:CYS:HB3	2.38	0.48
1:H:75:TRP:HH2	1:H:128:LEU:HD13	1.78	0.48
1:H:138:ILE:HG21	1:H:149:ILE:CD1	2.43	0.48
1:C:206:THR:CG2	1:C:338:LEU:HD21	2.44	0.48
1:B:63:ILE:O	1:B:67:VAL:HG23	2.13	0.48
1:G:110:LEU:O	1:G:110:LEU:HD22	2.13	0.48
1:F:3:LYS:CB	1:F:4:LEU:HD12	2.43	0.48
1:A:185:LYS:HD2	1:A:185:LYS:C	2.34	0.48
1:C:208:VAL:CG2	1:C:213:LYS:HE2	2.44	0.48
1:E:13:LEU:HB3	1:E:86:HIS:CA	2.43	0.48
1:H:178:ASN:CG	1:H:181:ASP:HB2	2.34	0.48
1:G:119:PHE:CD1	1:G:119:PHE:N	2.81	0.48
1:D:7:LYS:HG2	1:D:111:TRP:CH2	2.48	0.48
1:E:342:ARG:HG2	1:E:342:ARG:NH1	2.24	0.48
1:B:142:HIS:N	1:B:143:PRO:CD	2.77	0.48
1:D:223:VAL:CG1	1:D:274:THR:HB	2.43	0.48
1:E:429:TYR:CE2	1:E:431:TYR:HA	2.48	0.48
1:A:142:HIS:N	1:A:143:PRO:CD	2.77	0.48
1:G:155:GLU:O	1:G:185:LYS:HE3	2.14	0.48
1:F:300:HIS:H	2:F:6432:NAD:H1D	1.78	0.48
1:G:48:ARG:HD2	1:G:119:PHE:HB2	1.96	0.48
1:F:28:MET:HB3	1:F:358:SER:HB2	1.94	0.48
1:G:249:LEU:HB3	1:H:188:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LYS:NZ	1:D:101:TRP:CE3	2.64	0.48
1:E:277:CYS:SG	1:E:278:VAL:N	2.86	0.48
1:H:183:VAL:HG21	1:H:431:TYR:CE1	2.48	0.48
1:H:223:VAL:HG23	2:H:8432:NAD:O2N	2.14	0.48
1:D:185:LYS:HD2	1:D:185:LYS:C	2.34	0.48
1:E:86:HIS:ND1	1:E:87:ALA:N	2.61	0.48
1:G:65:THR:O	1:G:69:LEU:HD13	2.14	0.48
1:A:308:LYS:HD2	1:A:308:LYS:H	1.78	0.48
1:C:224:GLY:HA2	1:C:274:THR:HG21	1.96	0.48
1:B:35:ARG:O	1:B:39:SER:HB2	2.14	0.48
1:G:60:ALA:O	1:G:64:GLU:HG3	2.13	0.48
1:A:304:GLU:HG2	1:A:304:GLU:H	1.46	0.48
1:G:55:MET:HG2	1:G:88:ALA:HB2	1.95	0.48
1:G:99:PHE:N	1:G:99:PHE:HD2	2.11	0.48
1:E:425:LYS:HG3	1:E:431:TYR:CZ	2.48	0.48
1:G:53:LEU:O	1:G:54:HIS:C	2.52	0.48
1:G:155:GLU:HB2	1:G:364:GLN:OE1	2.14	0.48
1:F:283:GLY:HA3	1:F:309:TRP:CE2	2.48	0.48
1:G:389:LEU:O	1:G:393:VAL:HG23	2.13	0.48
1:C:199:ILE:HG22	1:C:203:LYS:HG3	1.95	0.48
1:D:4:LEU:HD11	1:D:111:TRP:CZ2	2.49	0.48
1:F:74:ARG:HG3	1:F:119:PHE:CE2	2.49	0.48
1:F:72:GLU:OE2	1:F:120:LYS:HE3	2.14	0.48
1:E:408:LEU:HD21	1:E:416:LEU:HD12	1.96	0.48
1:H:127:ILE:HG23	1:H:134:LEU:CD1	2.43	0.48
1:E:152:ILE:HB	1:E:176:ALA:HB2	1.94	0.48
1:H:373:THR:HG22	1:H:374:HIS:CD2	2.48	0.48
1:F:385:LEU:HD12	1:F:386:PRO:HD2	1.96	0.48
1:G:24:ALA:O	1:G:28:MET:HG3	2.13	0.48
1:H:63:ILE:O	1:H:66:LEU:HB2	2.14	0.48
1:H:3:LYS:HD3	1:H:115:GLN:NE2	2.29	0.47
1:A:225:LYS:HZ3	1:A:250:GLN:HE22	1.62	0.47
1:H:138:ILE:HG22	1:H:146:LEU:CD1	2.44	0.47
1:G:169:ASN:CB	1:G:171:ILE:HG12	2.44	0.47
1:G:152:ILE:HG22	1:G:153:SER:N	2.28	0.47
1:C:141:LYS:HB3	1:C:142:HIS:ND1	2.29	0.47
1:E:161:HIS:CD2	1:E:165:LYS:HZ2	2.28	0.47
1:B:206:THR:CG2	1:B:338:LEU:HD21	2.44	0.47
1:C:249:LEU:O	1:C:253:MET:HG2	2.13	0.47
1:E:215:ALA:O	1:E:238:VAL:HA	2.14	0.47
1:H:210:ILE:HG22	1:H:236:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HG2	1:B:111:TRP:CH2	2.49	0.47
1:A:2:ASP:HB3	1:A:3:LYS:HE3	1.96	0.47
1:D:3:LYS:N	1:D:3:LYS:HE3	2.29	0.47
1:E:101:TRP:CD2	1:E:104:GLU:HG2	2.50	0.47
1:B:142:HIS:O	1:B:145:LEU:HG	2.14	0.47
1:C:142:HIS:N	1:C:143:PRO:CD	2.77	0.47
1:C:306:ASP:OD2	1:C:309:TRP:HB2	2.15	0.47
1:G:344:VAL:HG13	1:G:345:ASN:N	2.29	0.47
1:A:271:PHE:CE1	1:A:289:MET:HG2	2.49	0.47
1:G:221:GLY:HA3	2:G:7432:NAD:O5B	2.14	0.47
1:F:101:TRP:CZ2	1:F:108:GLU:OE2	2.67	0.47
1:F:2:ASP:C	1:F:3:LYS:HE3	2.34	0.47
1:F:4:LEU:CD1	1:F:99:PHE:HE1	2.15	0.47
1:D:275:THR:CG2	1:D:276:GLY:N	2.76	0.47
1:H:153:SER:CB	1:H:364:GLN:HE22	2.26	0.47
1:E:319:ASN:HA	1:E:325:ASP:OD2	2.15	0.47
1:G:79:ASN:HB3	1:G:82:SER:HB3	1.95	0.47
1:G:279:ASP:N	1:G:279:ASP:OD1	2.47	0.47
1:E:214:VAL:HG11	1:E:267:GLU:HG2	1.96	0.47
1:C:429:TYR:CE2	1:C:431:TYR:HA	2.49	0.47
1:G:31:LEU:O	1:G:35:ARG:HG3	2.13	0.47
1:D:205:ALA:HB1	1:D:338:LEU:HD22	1.96	0.47
1:A:6:TYR:HB2	1:A:98:VAL:O	2.14	0.47
1:G:296:CYS:HB3	1:G:338:LEU:HB2	1.97	0.47
1:F:386:PRO:HG2	1:F:389:LEU:CD1	2.43	0.47
1:D:365:VAL:O	1:D:369:ILE:HG13	2.14	0.47
1:C:91:ILE:HG23	1:C:96:ILE:HB	1.95	0.47
1:G:281:ILE:HD13	1:G:289:MET:HE1	1.96	0.47
1:E:2:ASP:HB3	1:E:3:LYS:H	1.43	0.47
1:A:111:TRP:O	1:A:115:GLN:HG2	2.15	0.47
1:C:4:LEU:HD11	1:C:111:TRP:CZ2	2.49	0.47
1:H:7:LYS:HZ1	1:H:100:ALA:CA	2.28	0.47
1:G:101:TRP:O	1:G:104:GLU:HG2	2.13	0.47
1:H:198:LEU:HG	1:H:199:ILE:N	2.28	0.47
1:G:125:ASN:HA	1:G:149:ILE:HA	1.97	0.47
1:G:419:PRO:HG2	1:G:422:GLY:HA3	1.97	0.47
1:D:44:LEU:HB3	1:D:71:ALA:HB2	1.95	0.47
1:D:304:GLU:H	1:D:304:GLU:HG2	1.43	0.47
1:H:200:ASP:CG	1:H:204:ARG:HH21	2.17	0.47
1:H:33:ARG:O	1:H:33:ARG:NH2	2.47	0.47
1:B:3:LYS:H	1:B:3:LYS:CE	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:NH1	1:A:115:GLN:O	2.48	0.47
1:H:55:MET:CB	1:H:83:THR:HG23	2.37	0.47
1:H:85:ASP:OD2	1:H:101:TRP:HA	2.15	0.47
1:E:430:ARG:CZ	1:F:183:VAL:HG22	2.44	0.47
1:F:430:ARG:O	1:F:431:TYR:C	2.52	0.47
1:D:278:VAL:HA	1:D:303:VAL:O	2.13	0.47
1:B:430:ARG:HH11	1:B:430:ARG:HG3	1.80	0.47
1:G:308:LYS:O	1:G:311:ASN:N	2.48	0.47
1:E:342:ARG:O	1:E:343:LEU:C	2.52	0.47
1:F:167:MET:HE3	1:F:380:VAL:HG12	1.95	0.47
1:G:125:ASN:C	1:G:125:ASN:OD1	2.53	0.47
1:C:388:LYS:HG2	1:C:423:PRO:CG	2.45	0.47
1:G:152:ILE:CD1	1:G:174:VAL:HG22	2.45	0.47
1:G:152:ILE:HB	1:G:176:ALA:CB	2.44	0.47
1:C:167:MET:HE3	1:C:381:GLY:HA2	1.96	0.47
1:E:234:PHE:HE1	1:G:195:ARG:O	1.97	0.47
1:E:388:LYS:HD3	1:E:388:LYS:HA	1.70	0.47
1:G:218:ALA:HB3	1:G:273:THR:HA	1.96	0.47
1:H:379:PRO:HD2	1:H:383:HIS:CE1	2.50	0.47
1:B:4:LEU:HD11	1:B:111:TRP:CZ2	2.49	0.47
1:H:117:LEU:HD13	1:H:142:HIS:CD2	2.50	0.47
1:H:302:ASP:HB3	1:H:342:ARG:HA	1.96	0.47
1:E:307:VAL:N	1:E:308:LYS:HE3	2.27	0.47
1:E:57:VAL:H	1:E:84:GLN:NE2	2.13	0.47
1:G:53:LEU:HG	1:G:130:ASP:HB2	1.97	0.47
1:G:296:CYS:HB3	1:G:338:LEU:HD12	1.97	0.47
1:C:279:ASP:HA	1:C:282:LEU:HD11	1.96	0.47
1:H:177:ILE:HD13	1:H:385:LEU:CD1	2.45	0.47
1:D:334:ARG:O	1:D:335:ILE:HD13	2.14	0.47
1:D:7:LYS:HG2	1:D:111:TRP:HZ3	1.79	0.47
1:F:326:ARG:HH11	1:F:326:ARG:CG	2.16	0.47
1:H:42:LYS:O	1:H:45:LYS:HB3	2.15	0.47
1:F:141:LYS:HB3	1:F:142:HIS:CE1	2.50	0.47
1:A:39:SER:O	1:A:42:LYS:HG2	2.14	0.47
1:H:331:ASN:OD1	1:H:333:HIS:HB2	2.15	0.47
1:H:344:VAL:HG13	1:H:345:ASN:N	2.30	0.47
1:A:362:THR:HG22	1:A:393:VAL:HG22	1.97	0.47
1:F:38:TYR:HB3	1:F:43:PRO:CD	2.45	0.47
1:E:7:LYS:HZ1	1:E:100:ALA:N	2.11	0.47
1:H:142:HIS:HB3	1:H:145:LEU:HG	1.97	0.47
1:B:124:LEU:HD11	1:B:138:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:VAL:CG1	1:C:303:VAL:HB	2.44	0.47
1:C:388:LYS:HG2	1:C:423:PRO:CD	2.45	0.47
1:B:208:VAL:CG2	1:B:213:LYS:HE2	2.45	0.47
1:E:57:VAL:O	1:E:61:VAL:HG23	2.15	0.47
1:F:206:THR:HG21	1:F:294:ILE:HD13	1.97	0.47
1:C:203:LYS:O	1:C:207:ASP:N	2.48	0.47
1:A:91:ILE:HG23	1:A:96:ILE:HB	1.97	0.47
1:D:271:PHE:CE1	1:D:289:MET:HG2	2.50	0.47
1:G:215:ALA:CB	1:G:231:LEU:HD22	2.44	0.47
1:D:208:VAL:HG22	1:D:213:LYS:HE2	1.97	0.46
1:C:243:ILE:HG21	1:D:408:LEU:CD1	2.44	0.46
1:F:344:VAL:CG1	1:F:345:ASN:N	2.77	0.46
1:D:203:LYS:O	1:D:207:ASP:N	2.47	0.46
1:A:79:ASN:HB3	1:A:82:SER:OG	2.14	0.46
1:H:80:ILE:HG13	1:H:81:PHE:CD1	2.50	0.46
1:G:243:ILE:HA	1:H:406:THR:O	2.14	0.46
1:C:33:ARG:NH1	1:C:37:MET:SD	2.87	0.46
1:D:74:ARG:NH1	1:D:115:GLN:O	2.48	0.46
1:D:429:TYR:CE2	1:D:431:TYR:HA	2.51	0.46
1:G:105:THR:O	1:G:109:TYR:N	2.46	0.46
1:E:7:LYS:HG2	1:E:111:TRP:CH2	2.51	0.46
1:E:33:ARG:O	1:E:37:MET:HG2	2.15	0.46
1:B:138:ILE:HG22	1:B:146:LEU:CD1	2.45	0.46
1:D:141:LYS:HB3	1:D:142:HIS:ND1	2.30	0.46
1:C:283:GLY:HA2	1:C:286:PHE:HB2	1.97	0.46
1:C:408:LEU:HD13	1:D:243:ILE:HG21	1.97	0.46
1:A:47:ALA:HA	1:A:125:ASN:HD21	1.81	0.46
1:G:33:ARG:NE	1:G:36:GLU:OE1	2.48	0.46
1:C:7:LYS:HG2	1:C:111:TRP:CH2	2.51	0.46
1:F:7:LYS:HZ1	1:F:100:ALA:CA	2.28	0.46
1:D:155:GLU:O	1:D:180:ASN:HB2	2.16	0.46
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.30	0.46
1:F:160:VAL:HG12	1:F:164:TYR:CE2	2.49	0.46
1:D:419:PRO:HB2	1:D:422:GLY:HA3	1.97	0.46
1:E:210:ILE:CG2	1:E:236:ALA:HB2	2.44	0.46
1:G:167:MET:HG3	1:G:381:GLY:HA2	1.97	0.46
1:B:48:ARG:HD2	1:B:119:PHE:CG	2.50	0.46
1:A:141:LYS:HB3	1:A:142:HIS:ND1	2.29	0.46
1:D:79:ASN:HB3	1:D:82:SER:HB3	1.97	0.46
1:A:425:LYS:HE2	1:B:247:ASN:ND2	2.29	0.46
1:G:267:GLU:HA	1:G:290:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:LEU:HD12	1:F:57:VAL:HG13	1.97	0.46
1:B:373:THR:O	1:B:375:PRO:HD3	2.14	0.46
1:G:430:ARG:CZ	1:H:183:VAL:HG22	2.44	0.46
1:H:183:VAL:HG21	1:H:431:TYR:CD1	2.50	0.46
1:E:138:ILE:HG22	1:E:146:LEU:HD13	1.96	0.46
1:G:162:ASN:ND2	1:G:163:LEU:N	2.63	0.46
1:E:419:PRO:HB2	1:E:422:GLY:N	2.29	0.46
1:G:154:GLU:OE2	1:G:154:GLU:HA	2.15	0.46
1:G:404:LYS:HB2	1:H:259:THR:HG22	1.98	0.46
1:D:206:THR:CG2	1:D:338:LEU:HD21	2.45	0.46
1:E:26:ASN:O	1:E:400:LYS:HE2	2.15	0.46
1:G:366:MET:O	1:G:370:GLU:HG2	2.15	0.46
1:C:3:LYS:H	1:C:3:LYS:HE3	1.80	0.46
1:H:105:THR:HG23	1:H:108:GLU:OE1	2.16	0.46
1:G:25:GLU:O	1:G:32:MET:HG2	2.16	0.46
1:G:223:VAL:O	1:G:226:GLY:N	2.48	0.46
1:E:110:LEU:HD22	1:E:114:GLU:HG3	1.97	0.46
1:H:93:LYS:HD3	1:H:93:LYS:HA	1.74	0.46
1:E:2:ASP:HB2	1:E:74:ARG:HH12	1.81	0.46
1:A:7:LYS:HG2	1:A:111:TRP:CH2	2.51	0.46
1:C:74:ARG:NH1	1:C:115:GLN:O	2.49	0.46
1:C:2:ASP:HB3	1:C:3:LYS:HE3	1.97	0.46
1:A:356:VAL:HB	1:C:209:MET:SD	2.55	0.46
1:A:127:ILE:HG21	1:A:135:THR:HG22	1.98	0.46
1:H:178:ASN:ND2	1:H:384:PHE:CE1	2.83	0.46
1:C:307:VAL:N	1:C:308:LYS:HE3	2.29	0.46
1:A:206:THR:CG2	1:A:338:LEU:HD21	2.46	0.46
1:G:157:THR:O	1:G:160:VAL:N	2.49	0.46
1:H:379:PRO:O	1:H:383:HIS:HE1	1.98	0.46
1:D:358:SER:HB3	1:D:397:HIS:NE2	2.31	0.46
1:H:65:THR:O	1:H:69:LEU:HD13	2.16	0.46
1:A:37:MET:CB	1:H:284:ARG:NH2	2.73	0.46
1:A:57:VAL:O	1:A:60:ALA:HB3	2.16	0.46
1:B:278:VAL:CG1	1:B:303:VAL:HB	2.41	0.46
1:H:52:CYS:HB3	1:H:129:ASP:OD1	2.14	0.46
1:G:242:GLU:OE1	1:G:243:ILE:N	2.45	0.46
1:B:91:ILE:HG23	1:B:96:ILE:HB	1.97	0.46
1:A:2:ASP:CB	1:A:74:ARG:HH12	2.26	0.46
1:H:7:LYS:HG2	1:H:111:TRP:HH2	1.77	0.46
1:E:373:THR:O	1:E:375:PRO:HD3	2.16	0.46
1:A:419:PRO:HB2	1:A:422:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PRO:HB2	1:B:422:GLY:HA3	1.98	0.46
1:G:190:ASN:N	1:G:190:ASN:OD1	2.49	0.46
1:A:283:GLY:HA2	1:A:286:PHE:HB2	1.97	0.46
1:G:224:GLY:HA2	1:G:274:THR:HG21	1.98	0.46
1:E:203:LYS:O	1:E:207:ASP:N	2.48	0.46
1:A:136:ASN:O	1:A:140:THR:HG23	2.16	0.46
1:H:416:LEU:HD13	1:H:418:MET:SD	2.56	0.46
1:F:92:ALA:HB2	1:F:98:VAL:CG1	2.46	0.46
1:G:3:LYS:HB2	1:G:4:LEU:CD1	2.46	0.46
1:E:105:THR:H	1:E:108:GLU:HB2	1.80	0.46
1:H:154:GLU:O	1:H:179:VAL:HB	2.16	0.46
1:C:184:THR:HA	1:C:188:PHE:CD1	2.51	0.46
1:G:34:MET:O	1:G:38:TYR:HD2	1.99	0.46
1:B:362:THR:O	1:B:366:MET:HG3	2.16	0.46
1:D:33:ARG:HE	1:D:36:GLU:CD	2.19	0.46
1:G:225:LYS:NZ	1:G:250:GLN:HE22	2.13	0.46
1:C:7:LYS:NZ	1:C:7:LYS:O	2.37	0.46
1:F:4:LEU:HD22	1:F:6:TYR:O	2.15	0.46
1:E:120:LYS:HG2	1:E:121:ASP:OD1	2.15	0.46
1:H:101:TRP:CZ2	1:H:108:GLU:OE1	2.61	0.46
1:E:342:ARG:NH1	1:E:342:ARG:CG	2.79	0.46
1:H:189:ASP:OD1	1:H:189:ASP:C	2.55	0.46
1:B:141:LYS:HB3	1:B:142:HIS:ND1	2.31	0.46
1:F:315:VAL:N	1:F:328:LEU:O	2.49	0.46
1:G:74:ARG:HB3	1:G:116:THR:HG22	1.96	0.46
1:F:350:MET:HB2	1:H:207:ASP:OD1	2.16	0.46
1:E:283:GLY:O	1:E:287:GLU:HG3	2.16	0.46
1:E:387:LYS:HA	1:E:390:ASP:HB2	1.97	0.46
1:B:99:PHE:N	1:B:99:PHE:CD2	2.84	0.45
1:B:275:THR:CG2	1:B:276:GLY:N	2.78	0.45
1:D:430:ARG:O	1:D:431:TYR:C	2.55	0.45
1:A:430:ARG:CA	1:B:430:ARG:HD3	2.44	0.45
1:G:258:VAL:HB	1:H:403:VAL:HG13	1.98	0.45
1:F:195:ARG:O	1:F:230:ALA:HB2	2.16	0.45
1:D:124:LEU:HD11	1:D:138:ILE:HD11	1.98	0.45
1:E:152:ILE:HG13	1:E:174:VAL:HG22	1.97	0.45
1:A:190:ASN:HB3	1:A:223:VAL:HG23	1.98	0.45
1:G:119:PHE:HD1	1:G:119:PHE:N	2.15	0.45
1:H:262:ASP:O	1:H:266:LYS:HE2	2.16	0.45
1:C:35:ARG:O	1:C:39:SER:HB2	2.16	0.45
1:B:304:GLU:HG2	1:B:304:GLU:H	1.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:PHE:CD1	1:H:188:PHE:N	2.84	0.45
1:F:57:VAL:HA	1:F:87:ALA:HB1	1.98	0.45
1:E:370:GLU:HG3	1:E:378:TYR:OH	2.16	0.45
1:E:48:ARG:HB3	1:E:119:PHE:CG	2.51	0.45
1:B:91:ILE:O	1:B:94:ALA:HB3	2.16	0.45
1:B:317:LYS:HD2	1:B:327:TYR:CE2	2.51	0.45
1:D:215:ALA:O	1:D:238:VAL:HA	2.17	0.45
1:C:334:ARG:O	1:C:335:ILE:HD13	2.17	0.45
1:E:92:ALA:HB2	1:E:98:VAL:CG1	2.45	0.45
1:H:32:MET:CE	1:H:35:ARG:HD2	2.46	0.45
1:C:430:ARG:CD	1:D:430:ARG:HA	2.35	0.45
1:G:83:THR:HG21	1:G:101:TRP:N	2.32	0.45
1:D:308:LYS:CE	1:D:308:LYS:H	2.30	0.45
1:A:308:LYS:CE	1:A:308:LYS:H	2.28	0.45
1:G:363:ASN:ND2	1:G:393:VAL:HG11	2.31	0.45
1:A:421:ASN:ND2	1:H:312:GLU:OE2	2.49	0.45
1:H:321:LYS:HD3	1:H:324:VAL:HG21	1.98	0.45
1:A:203:LYS:O	1:A:207:ASP:N	2.49	0.45
1:H:5:PRO:HB2	1:H:6:TYR:HD2	1.82	0.45
1:G:331:ASN:OD1	1:G:331:ASN:C	2.54	0.45
1:H:32:MET:HE3	1:H:35:ARG:HD2	1.99	0.45
1:D:33:ARG:NH1	1:D:37:MET:SD	2.89	0.45
1:B:74:ARG:NH1	1:B:115:GLN:O	2.49	0.45
1:F:6:TYR:HB2	1:F:98:VAL:O	2.16	0.45
1:E:10:ASP:HB3	1:E:13:LEU:HD22	1.98	0.45
1:E:292:ASP:N	1:E:334:ARG:O	2.49	0.45
1:G:278:VAL:HA	1:G:303:VAL:O	2.17	0.45
1:F:370:GLU:HB3	1:F:378:TYR:CE1	2.52	0.45
1:G:250:GLN:O	1:G:254:GLU:HG2	2.16	0.45
1:B:185:LYS:HD2	1:B:185:LYS:C	2.36	0.45
1:D:7:LYS:HE3	1:D:99:PHE:CB	2.46	0.45
1:H:9:ALA:HB2	1:H:101:TRP:HB2	1.97	0.45
1:E:37:MET:HG3	1:E:38:TYR:CE2	2.52	0.45
1:H:17:GLY:O	1:H:21:LEU:HB2	2.17	0.45
1:A:430:ARG:O	1:A:431:TYR:C	2.55	0.45
1:H:143:PRO:HA	1:H:146:LEU:HD13	1.98	0.45
1:F:356:VAL:HB	1:H:209:MET:SD	2.57	0.45
1:G:167:MET:HG2	1:G:172:LEU:CD1	2.46	0.45
1:G:153:SER:CB	1:G:368:GLN:NE2	2.79	0.45
1:F:66:LEU:HD11	1:F:128:LEU:CD1	2.46	0.45
1:B:178:ASN:HD21	1:B:181:ASP:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:PHE:O	1:E:192:TYR:HB2	2.16	0.45
1:F:208:VAL:HG11	1:F:294:ILE:HD12	1.98	0.45
1:C:369:ILE:O	1:C:373:THR:HB	2.17	0.45
1:B:7:LYS:HE3	1:B:99:PHE:CB	2.46	0.45
1:D:2:ASP:HB3	1:D:3:LYS:H	1.57	0.45
1:F:74:ARG:NH1	1:F:115:GLN:O	2.49	0.45
1:D:171:ILE:O	1:D:173:LYS:HG2	2.15	0.45
1:B:308:LYS:HD2	1:B:308:LYS:H	1.80	0.45
1:G:155:GLU:O	1:G:180:ASN:HB2	2.16	0.45
1:E:177:ILE:HD13	1:E:385:LEU:CD1	2.47	0.45
1:G:74:ARG:HD2	1:G:119:PHE:CD1	2.51	0.45
1:H:60:ALA:O	1:H:64:GLU:HG3	2.16	0.45
1:F:410:GLU:O	1:F:414:GLN:HG2	2.16	0.45
1:A:175:PRO:HB3	1:A:379:PRO:O	2.16	0.45
1:E:302:ASP:CG	1:E:302:ASP:O	2.55	0.45
1:C:7:LYS:HG2	1:C:111:TRP:HZ3	1.82	0.45
1:D:287:GLU:HG3	1:D:309:TRP:CZ2	2.52	0.45
1:H:172:LEU:HD22	1:H:174:VAL:H	1.81	0.45
1:G:91:ILE:CG2	1:G:96:ILE:HB	2.45	0.45
1:B:363:ASN:ND2	1:B:393:VAL:HG21	2.32	0.45
1:A:162:ASN:O	1:A:166:MET:HG3	2.16	0.45
1:E:291:ASP:HA	1:E:333:HIS:HB3	1.98	0.45
1:G:302:ASP:OD1	1:G:342:ARG:NH1	2.50	0.45
1:H:419:PRO:HG2	1:H:422:GLY:HA3	1.99	0.45
1:F:198:LEU:HD22	1:F:227:CYS:CB	2.36	0.45
1:A:430:ARG:HD3	1:B:430:ARG:CA	2.40	0.45
1:H:124:LEU:HD11	1:H:138:ILE:HD11	1.98	0.45
1:G:143:PRO:HA	1:G:146:LEU:HD22	1.99	0.45
1:E:13:LEU:HB3	1:E:86:HIS:CB	2.46	0.45
1:B:209:MET:HB2	1:D:353:PRO:CB	2.45	0.45
1:E:18:ARG:NH1	1:E:21:LEU:HD22	2.32	0.45
1:C:413:ALA:HB1	1:C:418:MET:O	2.16	0.45
1:B:271:PHE:CE1	1:B:289:MET:HG2	2.51	0.45
1:H:47:ALA:HA	1:H:125:ASN:HD21	1.82	0.45
1:F:119:PHE:CB	1:F:120:LYS:HE2	2.41	0.45
1:B:225:LYS:NZ	1:B:250:GLN:NE2	2.65	0.45
1:B:307:VAL:H	1:B:308:LYS:HE3	1.81	0.45
1:G:155:GLU:OE2	1:G:360:SER:HB3	2.17	0.45
1:G:265:CYS:SG	1:G:288:GLN:HG2	2.56	0.45
1:B:104:GLU:OE1	1:B:109:TYR:HA	2.16	0.45
1:D:91:ILE:HG23	1:D:96:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:TYR:OH	1:F:303:VAL:HG21	2.17	0.45
1:C:430:ARG:CZ	1:D:183:VAL:HG22	2.47	0.45
1:A:275:THR:CG2	1:A:276:GLY:N	2.80	0.45
1:E:7:LYS:CE	1:E:101:TRP:CE3	3.00	0.45
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.31	0.45
1:E:55:MET:CE	1:E:88:ALA:HA	2.47	0.45
1:G:183:VAL:HG21	1:G:431:TYR:CE1	2.52	0.45
1:A:224:GLY:HA2	1:A:274:THR:HG21	1.99	0.45
1:E:24:ALA:O	1:E:28:MET:HG3	2.17	0.45
1:E:283:GLY:HA2	1:E:286:PHE:HD2	1.82	0.45
1:H:321:LYS:HG2	1:H:324:VAL:HG23	1.99	0.45
1:F:240:ILE:O	1:F:258:VAL:HA	2.16	0.45
1:H:316:GLU:HB3	1:H:328:LEU:HB3	1.98	0.45
1:F:31:LEU:CD1	1:F:61:VAL:HG12	2.47	0.45
1:F:3:LYS:HB2	1:F:4:LEU:CD1	2.45	0.44
1:G:7:LYS:CD	1:G:111:TRP:HZ3	2.30	0.44
1:G:183:VAL:HG11	1:H:246:ILE:HG21	1.98	0.44
1:H:119:PHE:N	1:H:119:PHE:CD1	2.85	0.44
1:B:208:VAL:HG22	1:B:213:LYS:HE2	1.98	0.44
1:B:419:PRO:HG2	1:B:422:GLY:HA3	1.99	0.44
1:F:5:PRO:O	1:F:97:PRO:HA	2.17	0.44
1:E:328:LEU:C	1:E:328:LEU:HD12	2.38	0.44
1:E:101:TRP:CE2	1:E:104:GLU:HG2	2.52	0.44
1:E:7:LYS:NZ	1:E:100:ALA:N	2.64	0.44
1:C:214:VAL:H	1:C:269:ASN:ND2	2.10	0.44
1:A:57:VAL:H	1:A:84:GLN:HE22	1.65	0.44
1:F:419:PRO:HG2	1:F:422:GLY:HA3	1.99	0.44
1:F:154:GLU:HB2	1:F:163:LEU:CD1	2.46	0.44
1:F:353:PRO:O	1:F:357:MET:HG2	2.16	0.44
1:A:81:PHE:CE2	1:A:342:ARG:HG3	2.52	0.44
1:B:350:MET:HB2	1:D:207:ASP:OD1	2.16	0.44
1:G:144:GLN:HE21	1:G:144:GLN:HB2	1.57	0.44
1:E:189:ASP:OD1	1:E:352:HIS:CE1	2.70	0.44
1:D:119:PHE:HB3	1:D:120:LYS:HE2	2.00	0.44
1:H:7:LYS:HD3	1:H:111:TRP:CZ3	2.52	0.44
1:A:208:VAL:HG22	1:A:213:LYS:HE2	1.99	0.44
1:B:430:ARG:O	1:B:431:TYR:C	2.55	0.44
1:G:183:VAL:HG11	1:G:431:TYR:CG	2.52	0.44
1:H:185:LYS:CD	1:H:185:LYS:C	2.85	0.44
1:C:317:LYS:HD2	1:C:327:TYR:CE2	2.52	0.44
1:F:171:ILE:O	1:F:173:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ALA:O	1:C:28:MET:HG3	2.17	0.44
1:F:227:CYS:SG	1:F:274:THR:HG21	2.58	0.44
1:A:182:SER:HB2	1:A:185:LYS:HB2	1.99	0.44
1:B:430:ARG:NH1	1:B:430:ARG:HG3	2.32	0.44
1:H:238:VAL:HG12	1:H:240:ILE:HD12	2.00	0.44
1:F:51:GLY:HA3	1:F:75:TRP:CZ3	2.53	0.44
1:C:178:ASN:ND2	1:C:181:ASP:HB2	2.33	0.44
1:G:33:ARG:NH1	1:G:33:ARG:CG	2.78	0.44
1:G:321:LYS:O	1:G:322:PRO:C	2.56	0.44
1:H:275:THR:HG22	1:H:277:CYS:HB2	1.98	0.44
1:C:208:VAL:HG22	1:C:213:LYS:HE2	1.98	0.44
1:G:430:ARG:NE	1:H:183:VAL:HG22	2.32	0.44
1:B:57:VAL:H	1:B:84:GLN:HE22	1.61	0.44
1:H:336:ILE:HG22	1:H:338:LEU:CD2	2.48	0.44
1:C:205:ALA:HB1	1:C:338:LEU:HD22	1.99	0.44
1:F:58:GLU:OE2	3:F:6433:DEA:N6	2.47	0.44
1:E:74:ARG:NH1	1:E:115:GLN:O	2.48	0.44
1:F:48:ARG:HA	1:F:72:GLU:HB3	2.00	0.44
1:F:203:LYS:O	1:F:207:ASP:N	2.49	0.44
1:H:160:VAL:HG21	1:H:180:ASN:HB3	2.00	0.44
1:G:172:LEU:HD22	1:G:174:VAL:H	1.83	0.44
1:A:183:VAL:HG11	1:B:246:ILE:HG21	1.99	0.44
1:G:82:SER:HB2	1:G:346:LEU:HD22	1.99	0.44
1:E:49:ILE:HB	1:E:73:VAL:HG22	2.00	0.44
1:C:81:PHE:CE2	1:C:342:ARG:HG3	2.52	0.44
1:F:33:ARG:CG	1:F:33:ARG:NH1	2.56	0.44
1:G:3:LYS:HD2	1:G:115:GLN:OE1	2.18	0.44
1:H:17:GLY:O	1:H:21:LEU:HD13	2.18	0.44
1:G:62:LEU:HD22	1:G:361:PHE:CD1	2.52	0.44
1:C:308:LYS:CE	1:C:308:LYS:H	2.29	0.44
1:G:57:VAL:HG23	1:G:84:GLN:NE2	2.32	0.44
1:D:3:LYS:HE3	1:D:3:LYS:H	1.82	0.44
1:A:246:ILE:HG21	1:B:183:VAL:HG11	1.99	0.44
1:H:214:VAL:HG13	1:H:237:ARG:O	2.17	0.44
1:B:278:VAL:HA	1:B:303:VAL:O	2.17	0.44
1:G:58:GLU:HB3	1:G:361:PHE:HE2	1.82	0.44
1:H:91:ILE:CG2	1:H:96:ILE:HB	2.48	0.44
1:C:363:ASN:ND2	1:C:393:VAL:HG21	2.32	0.44
1:A:164:TYR:CZ	1:A:382:VAL:HG21	2.53	0.44
1:B:302:ASP:CG	1:B:302:ASP:O	2.55	0.44
1:G:11:ILE:HD12	1:G:11:ILE:HA	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:ARG:HE	1:G:36:GLU:CD	2.20	0.44
1:A:3:LYS:N	1:A:3:LYS:HE3	2.32	0.44
1:E:7:LYS:HZ1	1:E:100:ALA:C	2.21	0.44
1:D:419:PRO:HG2	1:D:422:GLY:HA3	2.00	0.44
1:G:63:ILE:HG21	1:G:96:ILE:HG21	2.00	0.44
1:B:160:VAL:HG21	1:B:178:ASN:OD1	2.17	0.44
1:C:358:SER:CB	1:C:397:HIS:NE2	2.80	0.44
1:H:200:ASP:O	1:H:204:ARG:HB2	2.18	0.44
1:A:315:VAL:HG23	1:A:330:LYS:HG2	1.99	0.44
1:H:176:ALA:O	1:H:382:VAL:HA	2.17	0.44
1:D:35:ARG:O	1:D:39:SER:HB2	2.18	0.43
1:A:7:LYS:NZ	1:A:7:LYS:O	2.36	0.43
1:C:387:LYS:HE2	1:C:431:TYR:OH	2.17	0.43
1:D:277:CYS:SG	1:D:278:VAL:N	2.91	0.43
1:F:209:MET:HB2	1:H:353:PRO:HB2	1.99	0.43
1:E:185:LYS:C	1:E:185:LYS:HD2	2.38	0.43
1:F:419:PRO:HB2	1:F:422:GLY:CA	2.48	0.43
1:D:287:GLU:HG3	1:D:309:TRP:CH2	2.52	0.43
1:F:34:MET:CE	1:F:366:MET:HG3	2.48	0.43
1:D:265:CYS:HA	1:D:271:PHE:CE2	2.54	0.43
1:B:30:GLY:HA3	1:B:362:THR:OG1	2.18	0.43
1:A:199:ILE:HG22	1:A:203:LYS:HG3	2.00	0.43
1:H:47:ALA:HB2	1:H:372:TRP:CE2	2.52	0.43
1:C:304:GLU:H	1:C:304:GLU:HG2	1.40	0.43
1:C:32:MET:O	1:C:36:GLU:HG3	2.18	0.43
1:H:386:PRO:CG	1:H:389:LEU:HD12	2.32	0.43
1:C:120:LYS:HE2	1:C:120:LYS:N	2.18	0.43
1:G:142:HIS:N	1:G:143:PRO:CD	2.81	0.43
1:G:35:ARG:HE	1:G:65:THR:CA	2.30	0.43
1:F:388:LYS:HG2	1:F:423:PRO:CG	2.47	0.43
1:B:388:LYS:HG2	1:B:423:PRO:HD3	1.99	0.43
1:C:152:ILE:HG13	1:C:174:VAL:HG22	2.00	0.43
1:G:6:TYR:HB2	1:G:98:VAL:O	2.18	0.43
1:E:194:CYS:SG	1:E:223:VAL:HG13	2.58	0.43
1:D:302:ASP:O	1:D:302:ASP:CG	2.56	0.43
1:H:33:ARG:O	1:H:37:MET:CG	2.66	0.43
1:A:101:TRP:HZ2	1:A:108:GLU:CD	2.22	0.43
1:C:101:TRP:HZ2	1:C:108:GLU:CD	2.20	0.43
1:C:180:ASN:C	1:C:180:ASN:ND2	2.71	0.43
1:G:198:LEU:HD22	1:G:227:CYS:HB3	1.99	0.43
1:G:79:ASN:HB3	1:G:82:SER:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:VAL:HB	1:G:279:ASP:OD1	2.19	0.43
1:D:388:LYS:HG2	1:D:423:PRO:HD3	1.98	0.43
1:E:50:ALA:HB3	1:E:124:LEU:HD12	2.01	0.43
1:E:47:ALA:HB2	1:E:372:TRP:CE2	2.53	0.43
1:E:151:GLY:HA3	1:E:371:LEU:HG	2.01	0.43
1:D:363:ASN:ND2	1:D:393:VAL:HG21	2.34	0.43
1:A:425:LYS:HE2	1:B:247:ASN:HD21	1.83	0.43
1:C:331:ASN:OD1	1:C:333:HIS:HB2	2.19	0.43
1:C:271:PHE:CE1	1:C:289:MET:HG2	2.53	0.43
1:E:144:GLN:HE21	1:E:144:GLN:HB2	1.58	0.43
1:B:3:LYS:HE3	1:B:3:LYS:N	2.31	0.43
1:C:4:LEU:HD13	1:C:99:PHE:CE1	2.48	0.43
1:G:308:LYS:H	1:G:308:LYS:CE	2.31	0.43
1:E:180:ASN:O	1:E:180:ASN:ND2	2.52	0.43
1:G:180:ASN:HA	1:G:185:LYS:HG3	1.99	0.43
1:E:329:LEU:C	1:E:331:ASN:N	2.71	0.43
1:A:6:TYR:OH	1:A:11:ILE:HD13	2.18	0.43
1:C:365:VAL:O	1:C:369:ILE:HG13	2.19	0.43
1:G:411:LYS:NZ	1:H:279:ASP:OD2	2.48	0.43
1:A:144:GLN:HE21	1:A:144:GLN:HB2	1.70	0.43
1:D:32:MET:O	1:D:35:ARG:HB2	2.18	0.43
1:B:180:ASN:HA	1:B:185:LYS:CE	2.33	0.43
1:A:409:THR:H	1:A:412:GLN:HE21	1.66	0.43
1:H:3:LYS:HB2	1:H:4:LEU:HD12	2.01	0.43
1:H:2:ASP:HA	1:H:3:LYS:HE3	2.00	0.43
1:G:101:TRP:HZ2	1:G:108:GLU:OE1	2.02	0.43
1:G:210:ILE:HB	1:G:234:PHE:HB3	2.00	0.43
1:E:4:LEU:HD11	1:E:111:TRP:HZ2	1.82	0.43
1:B:183:VAL:HG21	1:B:431:TYR:CE1	2.53	0.43
1:H:143:PRO:O	1:H:146:LEU:HB2	2.19	0.43
1:G:152:ILE:HG13	1:G:174:VAL:HG21	2.01	0.43
1:A:119:PHE:N	1:A:119:PHE:CD1	2.86	0.43
1:C:188:PHE:HA	1:C:192:TYR:CD2	2.53	0.43
1:H:336:ILE:HG22	1:H:338:LEU:HD23	2.01	0.43
1:B:244:ASP:HB3	1:B:247:ASN:HB2	2.00	0.43
1:D:54:HIS:CE1	1:D:78:CYS:SG	3.12	0.43
1:B:162:ASN:O	1:B:166:MET:HG3	2.18	0.43
1:G:275:THR:O	1:G:304:GLU:OE2	2.36	0.43
1:A:7:LYS:HE3	1:A:99:PHE:C	2.39	0.43
1:C:2:ASP:HB3	1:C:3:LYS:H	1.55	0.43
1:C:3:LYS:N	1:C:3:LYS:HE3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:VAL:HG21	1:C:431:TYR:CE1	2.54	0.43
1:F:209:MET:O	1:F:213:LYS:HD2	2.18	0.43
1:G:387:LYS:HE2	1:G:431:TYR:OH	2.18	0.43
1:H:58:GLU:C	1:H:361:PHE:HE2	2.22	0.43
1:E:161:HIS:CD2	1:E:161:HIS:C	2.91	0.43
1:B:39:SER:O	1:B:42:LYS:HG2	2.18	0.43
1:A:26:ASN:O	1:A:400:LYS:HE2	2.18	0.43
1:D:310:LEU:HB3	1:D:327:TYR:CE2	2.53	0.43
1:D:101:TRP:HZ2	1:D:108:GLU:OE1	2.02	0.43
1:E:247:ASN:HD21	1:F:425:LYS:HE2	1.83	0.43
1:A:275:THR:HG22	1:A:276:GLY:H	1.82	0.43
1:A:415:TYR:OH	1:B:303:VAL:HG21	2.18	0.43
1:H:232:ARG:CG	1:H:232:ARG:HH11	2.25	0.43
1:C:419:PRO:HB2	1:C:422:GLY:HA3	2.01	0.43
1:C:142:HIS:HB3	1:C:145:LEU:HG	2.00	0.43
1:E:169:ASN:HB2	1:E:171:ILE:HG12	2.00	0.43
1:G:130:ASP:OD1	1:G:156:THR:HB	2.18	0.43
1:D:208:VAL:HG22	1:D:209:MET:N	2.33	0.43
1:B:101:TRP:HZ2	1:B:108:GLU:OE1	2.01	0.43
1:C:430:ARG:HA	1:D:430:ARG:CD	2.40	0.43
1:D:124:LEU:HD11	1:D:138:ILE:CD1	2.48	0.43
1:G:91:ILE:HA	1:G:91:ILE:HD13	1.76	0.43
1:E:273:THR:OG1	1:E:297:ASN:OD1	2.33	0.43
1:G:375:PRO:C	1:G:377:LYS:H	2.21	0.43
1:F:257:GLU:HG3	1:G:237:ARG:CZ	2.48	0.43
1:B:201:GLY:HA2	1:B:349:ALA:HB2	2.00	0.43
1:C:35:ARG:NH2	1:C:64:GLU:HB2	2.33	0.43
1:A:334:ARG:O	1:A:335:ILE:HD13	2.19	0.43
1:C:345:ASN:O	1:C:349:ALA:HB3	2.18	0.43
1:A:33:ARG:HE	1:A:36:GLU:CD	2.22	0.43
1:B:182:SER:HB2	1:B:185:LYS:HB2	2.01	0.43
1:B:2:ASP:HB3	1:B:3:LYS:H	1.62	0.43
1:D:99:PHE:N	1:D:99:PHE:CD2	2.86	0.43
1:H:7:LYS:CD	1:H:101:TRP:HZ3	2.32	0.43
1:G:83:THR:HG21	1:G:100:ALA:C	2.39	0.43
1:F:419:PRO:HB2	1:F:422:GLY:HA3	1.99	0.43
1:C:167:MET:HE1	1:C:380:VAL:O	2.19	0.43
1:H:62:LEU:O	1:H:66:LEU:HG	2.19	0.43
1:H:391:GLU:OE2	1:H:423:PRO:HA	2.18	0.43
1:B:176:ALA:O	1:B:382:VAL:HA	2.19	0.43
1:B:4:LEU:HD11	1:B:111:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:THR:HG23	1:C:108:GLU:OE1	2.19	0.43
1:C:7:LYS:HE3	1:C:99:PHE:CB	2.47	0.43
1:C:430:ARG:O	1:C:431:TYR:C	2.57	0.43
1:G:105:THR:N	1:G:108:GLU:HB2	2.29	0.43
1:G:209:MET:O	1:G:213:LYS:HD2	2.19	0.43
1:F:183:VAL:HG11	1:F:431:TYR:CG	2.54	0.43
1:A:180:ASN:HA	1:A:185:LYS:CE	2.42	0.43
1:A:232:ARG:CG	1:A:232:ARG:HH11	2.31	0.43
1:A:388:LYS:HG2	1:A:423:PRO:CG	2.48	0.43
1:E:126:MET:HE2	1:E:372:TRP:N	2.34	0.43
1:G:287:GLU:HG3	1:G:309:TRP:CH2	2.54	0.43
1:E:91:ILE:O	1:E:94:ALA:HB3	2.19	0.43
1:D:119:PHE:N	1:D:119:PHE:CD1	2.87	0.42
1:C:182:SER:HB2	1:C:185:LYS:HB2	2.01	0.42
1:G:167:MET:HE2	1:G:172:LEU:HB3	2.01	0.42
1:G:74:ARG:HD2	1:G:119:PHE:CE1	2.54	0.42
1:B:297:ASN:OD1	1:B:304:GLU:HG3	2.18	0.42
1:D:163:LEU:HD11	1:D:176:ALA:HB1	2.01	0.42
1:C:105:THR:H	1:C:108:GLU:HB2	1.84	0.42
1:A:57:VAL:HG23	1:A:84:GLN:NE2	2.34	0.42
1:H:209:MET:O	1:H:213:LYS:HD2	2.19	0.42
1:D:142:HIS:HB3	1:D:145:LEU:HG	2.01	0.42
1:C:142:HIS:O	1:C:145:LEU:HG	2.19	0.42
1:G:178:ASN:CG	1:G:181:ASP:HB2	2.39	0.42
1:F:225:LYS:NZ	1:F:250:GLN:HE22	2.17	0.42
1:G:266:LYS:HG2	1:G:288:GLN:HG2	2.00	0.42
1:G:286:PHE:C	1:G:288:GLN:N	2.72	0.42
1:C:44:LEU:HB3	1:C:71:ALA:HB2	2.01	0.42
1:H:315:VAL:HG23	1:H:330:LYS:HG2	2.01	0.42
1:G:209:MET:HE2	1:G:211:ALA:HB3	2.01	0.42
1:A:208:VAL:HG22	1:A:209:MET:N	2.34	0.42
1:E:342:ARG:HH11	1:E:342:ARG:CG	2.21	0.42
1:F:196:GLU:HA	1:H:234:PHE:CE1	2.52	0.42
1:F:321:LYS:HB2	1:F:322:PRO:HD2	2.01	0.42
1:G:54:HIS:HB3	1:G:82:SER:OG	2.19	0.42
1:B:342:ARG:O	1:B:343:LEU:C	2.57	0.42
1:H:163:LEU:HD11	1:H:176:ALA:HB1	2.01	0.42
1:C:386:PRO:HG2	1:C:389:LEU:HG	2.01	0.42
1:E:415:TYR:CE1	1:F:278:VAL:HG13	2.53	0.42
1:B:3:LYS:CE	1:B:3:LYS:N	2.82	0.42
1:A:412:GLN:HG2	1:B:277:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ILE:HG23	1:F:134:LEU:CD1	2.50	0.42
1:C:154:GLU:HG2	1:C:160:VAL:N	2.33	0.42
1:A:79:ASN:HB3	1:A:82:SER:HB3	2.00	0.42
1:H:208:VAL:HG11	1:H:294:ILE:CD1	2.49	0.42
1:F:37:MET:HG2	1:F:37:MET:H	1.66	0.42
1:B:355:PHE:CZ	1:B:401:LEU:HD21	2.55	0.42
1:E:240:ILE:HD12	1:E:256:TYR:HB3	2.01	0.42
1:E:7:LYS:HZ1	1:E:100:ALA:CA	2.32	0.42
1:H:152:ILE:HG22	1:H:153:SER:N	2.34	0.42
1:G:153:SER:HB2	1:G:368:GLN:HE22	1.82	0.42
1:E:21:LEU:O	1:E:25:GLU:N	2.53	0.42
1:H:321:LYS:HG2	1:H:324:VAL:CG2	2.50	0.42
1:A:385:LEU:O	1:A:386:PRO:C	2.58	0.42
1:C:275:THR:CG2	1:C:276:GLY:H	2.32	0.42
1:F:7:LYS:NZ	1:F:101:TRP:CE3	2.65	0.42
1:H:3:LYS:N	1:H:3:LYS:CD	2.82	0.42
1:D:183:VAL:HG21	1:D:431:TYR:CE1	2.55	0.42
1:D:146:LEU:HA	1:D:146:LEU:HD12	1.89	0.42
1:B:225:LYS:HZ3	1:B:250:GLN:HE22	1.67	0.42
1:F:319:ASN:ND2	1:F:321:LYS:O	2.49	0.42
1:C:198:LEU:HD22	1:C:227:CYS:CB	2.49	0.42
1:E:326:ARG:HG3	1:E:336:ILE:HG12	2.00	0.42
1:G:188:PHE:HA	1:G:192:TYR:CD2	2.55	0.42
1:F:152:ILE:CG2	1:F:153:SER:N	2.82	0.42
1:E:221:GLY:O	1:E:225:LYS:HB2	2.19	0.42
1:G:187:LYS:HA	1:G:187:LYS:HD2	1.87	0.42
1:H:278:VAL:HA	1:H:303:VAL:O	2.18	0.42
1:F:2:ASP:OD2	1:F:118:HIS:HB2	2.20	0.42
1:B:365:VAL:O	1:B:369:ILE:HG13	2.20	0.42
1:G:425:LYS:HE2	1:G:429:TYR:CE2	2.54	0.42
1:G:430:ARG:CG	1:G:430:ARG:HH11	2.33	0.42
1:F:319:ASN:O	1:H:19:LYS:HE2	2.20	0.42
1:F:180:ASN:HA	1:F:185:LYS:HE3	2.02	0.42
1:G:300:HIS:HB2	2:G:7432:NAD:O2D	2.20	0.42
1:G:300:HIS:N	2:G:7432:NAD:H1D	2.34	0.42
1:B:32:MET:O	1:B:36:GLU:HG3	2.20	0.42
1:F:4:LEU:HD23	1:F:7:LYS:HB3	2.00	0.42
1:G:101:TRP:CH2	1:G:108:GLU:HB3	2.55	0.42
1:E:38:TYR:HB2	1:E:69:LEU:CD1	2.48	0.42
1:A:180:ASN:C	1:A:180:ASN:ND2	2.72	0.42
1:G:311:ASN:OD1	1:G:327:TYR:CE2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ILE:HG22	1:C:153:SER:N	2.35	0.42
1:H:216:VAL:HG21	1:H:271:PHE:CE2	2.54	0.42
1:G:116:THR:O	1:G:119:PHE:CE1	2.72	0.42
1:H:326:ARG:HD2	1:H:336:ILE:CG1	2.50	0.42
1:A:247:ASN:ND2	1:B:425:LYS:HE2	2.35	0.42
1:H:177:ILE:HD12	1:H:371:LEU:HD13	2.02	0.42
1:E:302:ASP:HB2	1:E:341:GLY:O	2.19	0.42
1:D:198:LEU:HD22	1:D:227:CYS:SG	2.59	0.42
1:C:242:GLU:O	1:D:406:THR:HB	2.20	0.42
1:B:4:LEU:HD13	1:B:99:PHE:CE1	2.48	0.42
1:B:7:LYS:HG2	1:B:111:TRP:HZ3	1.84	0.42
1:H:425:LYS:HD2	1:H:429:TYR:CE1	2.55	0.42
1:H:155:GLU:OE2	1:H:360:SER:HB3	2.20	0.42
1:E:257:GLU:HB2	1:H:237:ARG:NE	2.34	0.42
1:E:127:ILE:HG23	1:E:134:LEU:HD13	2.02	0.42
1:D:10:ASP:O	1:D:13:LEU:HB2	2.20	0.42
1:B:419:PRO:HB2	1:B:422:GLY:CA	2.50	0.42
1:A:184:THR:HA	1:A:188:PHE:CD1	2.55	0.42
1:F:272:VAL:HA	1:F:296:CYS:O	2.20	0.42
1:H:291:ASP:OD2	1:H:334:ARG:NH2	2.52	0.42
1:C:79:ASN:HB3	1:C:82:SER:OG	2.20	0.42
1:A:265:CYS:HA	1:A:271:PHE:CE2	2.55	0.42
1:A:331:ASN:OD1	1:A:333:HIS:HB2	2.20	0.42
1:H:410:GLU:O	1:H:414:GLN:CG	2.68	0.42
1:A:158:THR:O	1:A:161:HIS:HB3	2.19	0.42
1:D:185:LYS:O	1:D:189:ASP:HB3	2.20	0.42
1:H:180:ASN:HA	1:H:185:LYS:HG3	2.02	0.42
1:A:150:ARG:HE	1:A:150:ARG:HB2	1.67	0.42
1:G:178:ASN:OD1	1:G:178:ASN:C	2.59	0.42
1:F:373:THR:HG22	1:F:374:HIS:CE1	2.55	0.42
1:A:80:ILE:HD11	1:A:342:ARG:HE	1.85	0.42
1:F:316:GLU:O	1:F:328:LEU:N	2.49	0.42
1:F:53:LEU:HB2	1:F:75:TRP:HZ2	1.83	0.42
1:H:339:ALA:HB2	1:H:348:CYS:SG	2.59	0.42
1:G:249:LEU:HD13	1:H:398:LEU:CD1	2.50	0.41
1:B:7:LYS:CE	1:B:101:TRP:CE3	3.03	0.41
1:B:37:MET:H	1:B:37:MET:HG2	1.61	0.41
1:C:99:PHE:CD2	1:C:99:PHE:N	2.87	0.41
1:D:105:THR:OG1	1:D:108:GLU:HG3	2.20	0.41
1:E:278:VAL:HA	1:E:303:VAL:O	2.20	0.41
1:E:309:TRP:O	1:E:313:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:LYS:HG2	1:E:269:ASN:HB3	2.02	0.41
1:G:210:ILE:O	1:G:213:LYS:HB2	2.20	0.41
1:A:120:LYS:N	1:A:120:LYS:HE2	2.19	0.41
1:C:21:LEU:O	1:C:25:GLU:HG3	2.19	0.41
1:H:169:ASN:HB2	1:H:171:ILE:HG12	2.02	0.41
1:B:208:VAL:HG22	1:B:209:MET:N	2.35	0.41
1:C:223:VAL:CG1	1:C:274:THR:HB	2.50	0.41
1:G:53:LEU:O	1:G:77:SER:HA	2.20	0.41
1:B:287:GLU:HG3	1:B:309:TRP:CZ2	2.55	0.41
1:B:79:ASN:HB3	1:B:82:SER:HB3	2.02	0.41
1:F:28:MET:HG2	1:F:354:SER:O	2.19	0.41
1:A:92:ALA:HB2	1:A:98:VAL:CG1	2.50	0.41
1:E:249:LEU:O	1:E:253:MET:HG2	2.19	0.41
1:G:342:ARG:O	1:G:343:LEU:C	2.59	0.41
1:H:389:LEU:O	1:H:392:ALA:HB3	2.20	0.41
1:C:105:THR:OG1	1:C:108:GLU:HG3	2.20	0.41
1:F:111:TRP:O	1:F:115:GLN:HG2	2.20	0.41
1:G:203:LYS:HE2	1:G:210:ILE:HG12	2.02	0.41
1:E:375:PRO:C	1:E:377:LYS:H	2.23	0.41
1:G:388:LYS:HG2	1:G:423:PRO:HD3	2.02	0.41
1:F:80:ILE:O	1:F:103:GLY:N	2.47	0.41
1:H:142:HIS:N	1:H:143:PRO:CD	2.83	0.41
1:F:180:ASN:OD1	1:F:185:LYS:NZ	2.45	0.41
1:H:35:ARG:CG	1:H:65:THR:OG1	2.68	0.41
1:F:188:PHE:O	1:F:192:TYR:HB2	2.19	0.41
1:A:209:MET:SD	1:C:356:VAL:HB	2.60	0.41
1:G:183:VAL:CG1	1:H:246:ILE:HG21	2.50	0.41
1:H:154:GLU:HG3	1:H:160:VAL:CG2	2.50	0.41
1:H:138:ILE:CG2	1:H:146:LEU:HD12	2.50	0.41
1:F:139:HIS:ND1	1:F:146:LEU:HD11	2.36	0.41
1:C:131:GLY:HA3	1:C:300:HIS:NE2	2.35	0.41
1:H:31:LEU:HD21	1:H:361:PHE:CB	2.50	0.41
1:B:300:HIS:HA	1:B:343:LEU:HD11	2.03	0.41
1:E:188:PHE:O	1:E:356:VAL:HG21	2.19	0.41
1:F:296:CYS:HB2	1:F:344:VAL:HG21	2.02	0.41
1:B:388:LYS:HG2	1:B:423:PRO:HG3	2.02	0.41
1:F:27:GLU:O	1:F:355:PHE:HA	2.19	0.41
1:G:411:LYS:O	1:G:414:GLN:HB2	2.20	0.41
1:G:326:ARG:HH12	1:G:334:ARG:HD2	1.85	0.41
1:D:33:ARG:O	1:D:37:MET:HG2	2.21	0.41
1:E:2:ASP:HB2	1:E:74:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:THR:HG23	2:G:7432:NAD:C8A	2.51	0.41
1:B:27:GLU:C	1:B:29:PRO:HD3	2.40	0.41
1:H:4:LEU:HD11	1:H:111:TRP:CZ2	2.55	0.41
1:E:214:VAL:CG1	1:E:239:ILE:HD12	2.50	0.41
1:H:179:VAL:O	1:H:185:LYS:HG3	2.20	0.41
1:A:419:PRO:HB2	1:A:422:GLY:CA	2.49	0.41
1:B:352:HIS:CE1	2:B:2432:NAD:H4N	2.56	0.41
1:C:91:ILE:O	1:C:94:ALA:HB3	2.21	0.41
1:G:410:GLU:OE2	1:G:414:GLN:HG2	2.19	0.41
1:G:217:VAL:HA	1:G:272:VAL:O	2.19	0.41
1:H:158:THR:HG21	1:H:301:PHE:CD2	2.55	0.41
1:A:101:TRP:CZ2	1:A:108:GLU:CD	2.94	0.41
1:E:100:ALA:HA	1:E:104:GLU:OE2	2.20	0.41
1:H:42:LYS:N	1:H:43:PRO:CD	2.84	0.41
1:G:429:TYR:CE2	1:G:431:TYR:HA	2.55	0.41
1:H:308:LYS:N	1:H:308:LYS:CE	2.76	0.41
1:H:154:GLU:HG3	1:H:160:VAL:N	2.35	0.41
1:F:154:GLU:HG3	1:F:160:VAL:HG23	2.03	0.41
1:B:408:LEU:HA	1:B:408:LEU:HD12	1.91	0.41
1:G:215:ALA:HB2	1:G:231:LEU:HD22	2.02	0.41
1:F:212:GLY:N	1:F:235:GLY:O	2.53	0.41
1:D:81:PHE:CE2	1:D:342:ARG:HG3	2.55	0.41
1:H:144:GLN:H	1:H:144:GLN:CD	2.23	0.41
1:B:7:LYS:HE2	1:B:101:TRP:CZ3	2.54	0.41
1:C:2:ASP:CB	1:C:74:ARG:HH12	2.31	0.41
1:D:7:LYS:CE	1:D:101:TRP:CE3	3.04	0.41
1:E:213:LYS:HG2	1:E:269:ASN:CB	2.51	0.41
1:D:250:GLN:O	1:D:254:GLU:HG2	2.20	0.41
1:G:104:GLU:OE1	1:G:109:TYR:HA	2.20	0.41
1:D:57:VAL:O	1:D:60:ALA:HB3	2.20	0.41
1:H:128:LEU:HG	1:H:364:GLN:HE22	1.86	0.41
1:E:142:HIS:HB3	1:E:145:LEU:CD1	2.51	0.41
1:F:366:MET:HE1	1:F:393:VAL:HG23	2.01	0.41
1:G:48:ARG:HH21	1:G:122:GLY:C	2.24	0.41
1:A:362:THR:CG2	1:A:393:VAL:HG22	2.50	0.41
1:F:313:ASN:N	1:F:313:ASN:HD22	2.19	0.41
1:D:178:ASN:ND2	1:D:181:ASP:HB2	2.35	0.41
1:G:81:PHE:CD2	1:G:342:ARG:HG3	2.55	0.41
1:B:27:GLU:O	1:B:355:PHE:HA	2.20	0.41
1:A:2:ASP:CA	1:A:3:LYS:HE3	2.51	0.41
1:A:7:LYS:NZ	1:A:101:TRP:CE3	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ASN:O	1:E:330:LYS:HE3	2.21	0.41
1:C:150:ARG:HB2	1:C:150:ARG:HE	1.65	0.41
1:E:80:ILE:HB	1:E:104:GLU:O	2.21	0.41
1:B:175:PRO:HA	1:B:381:GLY:H	1.85	0.41
1:A:127:ILE:HD11	1:A:138:ILE:HD12	2.02	0.41
1:B:80:ILE:HD11	1:B:342:ARG:HE	1.86	0.41
1:E:125:ASN:ND2	1:E:372:TRP:CH2	2.89	0.41
1:B:206:THR:HG23	1:B:338:LEU:HD21	2.02	0.41
1:D:297:ASN:OD1	1:D:304:GLU:HG3	2.21	0.41
1:B:265:CYS:HA	1:B:271:PHE:CE2	2.55	0.41
1:H:297:ASN:OD1	1:H:298:ILE:N	2.54	0.41
1:F:11:ILE:O	1:F:11:ILE:HG13	2.20	0.41
1:H:29:PRO:HD2	1:H:397:HIS:HD2	1.84	0.41
1:D:32:MET:O	1:D:36:GLU:HG3	2.20	0.41
1:B:101:TRP:HZ2	1:B:108:GLU:CD	2.23	0.41
1:D:7:LYS:HE3	1:D:99:PHE:C	2.41	0.41
1:E:4:LEU:HD11	1:E:111:TRP:CH2	2.56	0.41
1:C:13:LEU:HD12	1:C:13:LEU:HA	1.94	0.41
1:E:53:LEU:HA	1:E:78:CYS:SG	2.60	0.41
1:G:58:GLU:HG3	1:G:354:SER:HA	2.01	0.41
1:G:152:ILE:HD12	1:G:174:VAL:HG22	2.03	0.41
1:D:378:TYR:HD2	1:D:383:HIS:ND1	2.18	0.41
1:F:362:THR:HG22	1:F:393:VAL:HG22	2.03	0.41
1:D:59:THR:O	1:D:63:ILE:HG13	2.21	0.41
1:G:278:VAL:HG22	1:H:415:TYR:CG	2.56	0.41
1:E:386:PRO:O	1:E:389:LEU:HB2	2.20	0.41
1:F:386:PRO:HG2	1:F:389:LEU:HG	2.03	0.41
1:B:344:VAL:HG13	1:B:345:ASN:N	2.36	0.41
1:D:79:ASN:HB3	1:D:82:SER:OG	2.20	0.41
1:B:59:THR:O	1:B:63:ILE:HG13	2.21	0.41
1:G:28:MET:HB3	1:G:358:SER:CB	2.51	0.41
1:D:91:ILE:CG2	1:D:96:ILE:HB	2.50	0.41
1:F:63:ILE:HD11	1:F:75:TRP:CG	2.55	0.41
1:D:30:GLY:HA3	1:D:362:THR:OG1	2.21	0.41
1:A:275:THR:HG21	1:A:277:CYS:HB3	2.03	0.41
1:E:55:MET:HE2	1:E:88:ALA:HA	2.03	0.41
1:B:430:ARG:NH2	4:B:9213:HOH:O	2.54	0.41
1:G:430:ARG:HD3	1:H:430:ARG:CA	2.44	0.41
1:D:326:ARG:HG2	1:D:326:ARG:HH11	1.86	0.41
1:H:137:LEU:O	1:H:141:LYS:HB2	2.21	0.41
1:F:195:ARG:O	1:H:234:PHE:HE1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ASP:OD2	1:G:135:THR:CG2	2.67	0.41
1:E:178:ASN:ND2	1:E:384:PHE:CE1	2.85	0.41
1:E:184:THR:HB	1:E:359:ASN:ND2	2.36	0.41
1:E:296:CYS:O	1:E:305:ILE:HD11	2.20	0.41
1:F:202:ILE:O	1:F:206:THR:HG23	2.20	0.41
1:E:124:LEU:HD23	1:E:124:LEU:O	2.21	0.41
1:A:337:LEU:HD22	1:A:338:LEU:N	2.35	0.41
1:D:337:LEU:HD22	1:D:338:LEU:N	2.36	0.41
1:C:35:ARG:HH22	1:C:64:GLU:HB2	1.84	0.41
1:G:164:TYR:CZ	1:G:382:VAL:HG21	2.55	0.41
1:G:40:ALA:O	1:G:42:LYS:HG2	2.21	0.41
1:D:339:ALA:HB2	1:D:348:CYS:SG	2.61	0.41
1:G:206:THR:OG1	1:G:208:VAL:HG12	2.20	0.41
1:F:361:PHE:O	1:F:365:VAL:HG23	2.21	0.41
1:B:180:ASN:ND2	1:B:180:ASN:C	2.75	0.41
1:C:101:TRP:CZ2	1:C:108:GLU:CD	2.94	0.41
1:D:7:LYS:HE2	1:D:101:TRP:CZ3	2.56	0.41
1:G:322:PRO:O	1:G:323:GLN:HB2	2.21	0.41
1:G:7:LYS:CE	1:G:101:TRP:CZ3	3.03	0.41
1:H:199:ILE:HG12	1:H:199:ILE:H	1.62	0.41
1:E:33:ARG:O	1:E:33:ARG:NH2	2.54	0.41
1:A:430:ARG:CD	1:B:430:ARG:HA	2.42	0.41
1:E:300:HIS:HA	1:E:343:LEU:CD1	2.50	0.41
1:D:13:LEU:HA	1:D:13:LEU:HD12	1.87	0.41
1:G:138:ILE:O	1:G:142:HIS:N	2.54	0.41
1:D:419:PRO:HB2	1:D:422:GLY:CA	2.51	0.41
1:A:124:LEU:HD11	1:A:138:ILE:CD1	2.51	0.41
1:E:160:VAL:HG11	1:E:178:ASN:ND2	2.35	0.41
1:A:167:MET:HE1	1:A:380:VAL:O	2.21	0.41
1:C:206:THR:HG23	1:C:338:LEU:HD21	2.03	0.41
1:H:279:ASP:OD1	1:H:279:ASP:N	2.54	0.41
1:D:386:PRO:O	1:D:389:LEU:HB2	2.21	0.41
1:F:91:ILE:O	1:F:94:ALA:HB3	2.21	0.41
1:H:399:GLY:O	1:H:402:ASN:N	2.49	0.41
1:G:113:ILE:HG22	1:G:137:LEU:HD23	2.02	0.41
1:D:3:LYS:O	1:D:4:LEU:C	2.59	0.40
1:F:101:TRP:O	1:F:104:GLU:HG3	2.21	0.40
1:E:408:LEU:HG	1:E:412:GLN:HB3	2.04	0.40
1:E:196:GLU:HA	1:G:234:PHE:CE1	2.56	0.40
1:E:44:LEU:HD12	1:E:69:LEU:CB	2.50	0.40
1:B:119:PHE:N	1:B:119:PHE:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LYS:CE	1:B:308:LYS:H	2.34	0.40
1:E:188:PHE:HA	1:E:192:TYR:HD2	1.85	0.40
1:H:44:LEU:CD1	1:H:71:ALA:HB2	2.49	0.40
1:F:343:LEU:HG	2:F:6432:NAD:N7N	2.36	0.40
1:F:51:GLY:HA3	1:F:75:TRP:CE3	2.56	0.40
1:C:178:ASN:C	1:C:178:ASN:OD1	2.58	0.40
1:D:32:MET:HA	1:D:35:ARG:HD2	2.03	0.40
1:A:37:MET:HB3	1:H:284:ARG:CZ	2.50	0.40
1:A:2:ASP:HB3	1:A:3:LYS:H	1.58	0.40
1:C:4:LEU:HD11	1:C:111:TRP:CH2	2.56	0.40
1:F:416:LEU:CB	1:F:418:MET:HG2	2.52	0.40
1:C:125:ASN:ND2	1:C:372:TRP:CH2	2.90	0.40
1:A:430:ARG:CZ	1:B:183:VAL:HG22	2.51	0.40
1:C:278:VAL:HA	1:C:303:VAL:O	2.22	0.40
1:A:142:HIS:O	1:A:145:LEU:HG	2.21	0.40
1:C:352:HIS:CE1	2:C:3432:NAD:H4N	2.57	0.40
1:B:152:ILE:HG22	1:B:153:SER:N	2.36	0.40
1:E:125:ASN:HA	1:E:148:GLY:O	2.22	0.40
1:G:5:PRO:O	1:G:6:TYR:HB3	2.22	0.40
1:F:19:LYS:HE2	1:H:319:ASN:O	2.22	0.40
1:A:247:ASN:HD21	1:B:425:LYS:HE2	1.86	0.40
1:D:369:ILE:O	1:D:373:THR:CB	2.69	0.40
1:G:243:ILE:HG22	1:H:406:THR:O	2.20	0.40
1:F:359:ASN:O	1:F:363:ASN:ND2	2.48	0.40
1:G:16:TRP:O	1:G:19:LYS:HB2	2.21	0.40
1:E:59:THR:HA	1:E:361:PHE:CE2	2.57	0.40
1:E:317:LYS:HD2	1:E:327:TYR:CE2	2.57	0.40
1:D:27:GLU:C	1:D:29:PRO:HD3	2.42	0.40
1:G:275:THR:CG2	1:G:277:CYS:H	2.17	0.40
1:G:249:LEU:HB3	1:H:188:PHE:HE2	1.85	0.40
1:D:387:LYS:HE2	1:D:431:TYR:OH	2.21	0.40
1:A:53:LEU:O	1:A:54:HIS:C	2.60	0.40
1:E:142:HIS:N	1:E:143:PRO:CD	2.83	0.40
1:G:35:ARG:HG2	1:G:65:THR:HG23	2.03	0.40
1:F:31:LEU:HD13	1:F:61:VAL:HG12	2.03	0.40
1:B:164:TYR:CZ	1:B:382:VAL:HG21	2.56	0.40
1:F:32:MET:O	1:F:36:GLU:HG3	2.21	0.40
1:F:13:LEU:HB3	1:F:86:HIS:HA	2.03	0.40
1:A:3:LYS:O	1:A:4:LEU:C	2.60	0.40
1:G:4:LEU:CD1	1:G:99:PHE:HE1	2.33	0.40
1:B:124:LEU:HD11	1:B:138:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:ASP:OD1	1:E:130:ASP:N	2.53	0.40
1:C:225:LYS:NZ	1:C:250:GLN:NE2	2.70	0.40
1:F:146:LEU:HA	1:F:146:LEU:HD12	1.91	0.40
1:A:154:GLU:CG	1:A:160:VAL:HG23	2.51	0.40
1:A:160:VAL:HG21	1:A:178:ASN:OD1	2.22	0.40
1:A:342:ARG:O	1:A:343:LEU:C	2.59	0.40
1:D:232:ARG:HH11	1:D:232:ARG:CG	2.33	0.40
1:A:358:SER:CB	1:A:397:HIS:NE2	2.84	0.40
1:D:369:ILE:O	1:D:373:THR:HB	2.21	0.40
1:G:57:VAL:O	1:G:61:VAL:HG23	2.21	0.40
1:D:198:LEU:HD22	1:D:227:CYS:CB	2.52	0.40
1:C:92:ALA:HB2	1:C:98:VAL:CG1	2.52	0.40
1:B:144:GLN:HE21	1:B:144:GLN:HB2	1.55	0.40
1:G:81:PHE:HE2	1:G:342:ARG:HE	1.69	0.40
1:G:342:ARG:HG2	1:G:342:ARG:H	1.45	0.40
1:D:2:ASP:CB	1:D:3:LYS:HE3	2.52	0.40
1:F:57:VAL:CG2	1:F:87:ALA:HB2	2.51	0.40
1:B:369:ILE:O	1:B:373:THR:HB	2.21	0.40
1:B:254:GLU:OE1	1:B:254:GLU:HA	2.21	0.40
1:E:125:ASN:C	1:E:125:ASN:OD1	2.60	0.40
1:D:201:GLY:HA2	1:D:349:ALA:HB2	2.02	0.40
1:D:184:THR:HA	1:D:188:PHE:CD1	2.56	0.40
1:F:152:ILE:HB	1:F:176:ALA:CB	2.50	0.40
1:F:261:MET:C	1:F:263:GLU:N	2.74	0.40
1:F:279:ASP:HA	1:F:282:LEU:HD11	2.02	0.40
1:G:120:LYS:CD	1:G:120:LYS:H	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	428/431 (99%)	399 (93%)	27 (6%)	2 (0%)	34 76
1	B	428/431 (99%)	395 (92%)	30 (7%)	3 (1%)	26 70
1	C	428/431 (99%)	401 (94%)	23 (5%)	4 (1%)	21 64
1	D	428/431 (99%)	402 (94%)	25 (6%)	1 (0%)	52 88
1	E	428/431 (99%)	395 (92%)	28 (6%)	5 (1%)	16 56
1	F	428/431 (99%)	395 (92%)	29 (7%)	4 (1%)	21 64
1	G	428/431 (99%)	394 (92%)	30 (7%)	4 (1%)	21 64
1	H	428/431 (99%)	400 (94%)	27 (6%)	1 (0%)	52 88
All	All	3424/3448 (99%)	3181 (93%)	219 (6%)	24 (1%)	26 70

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	4	LEU
1	F	212	GLY
1	B	300	HIS
1	C	300	HIS
1	D	300	HIS
1	E	147	SER
1	G	4	LEU
1	G	376	ASP
1	A	300	HIS
1	C	376	ASP
1	E	300	HIS
1	E	376	ASP
1	E	375	PRO
1	F	422	GLY
1	G	157	THR
1	C	4	LEU
1	C	147	SER
1	G	97	PRO
1	A	4	LEU
1	B	4	LEU
1	E	422	GLY
1	F	97	PRO
1	B	422	GLY
1	H	422	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/353 (100%)	286 (81%)	67 (19%)	2	10
1	B	353/353 (100%)	287 (81%)	66 (19%)	2	10
1	C	353/353 (100%)	290 (82%)	63 (18%)	2	11
1	D	353/353 (100%)	284 (80%)	69 (20%)	2	9
1	E	353/353 (100%)	283 (80%)	70 (20%)	1	8
1	F	353/353 (100%)	285 (81%)	68 (19%)	2	9
1	G	353/353 (100%)	277 (78%)	76 (22%)	1	6
1	H	353/353 (100%)	268 (76%)	85 (24%)	1	4
All	All	2824/2824 (100%)	2260 (80%)	564 (20%)	1	8

All (564) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	LYS
1	A	4	LEU
1	A	7	LYS
1	A	11	ILE
1	A	13	LEU
1	A	27	GLU
1	A	33	ARG
1	A	37	MET
1	A	39	SER
1	A	41	SER
1	A	45	LYS
1	A	53	LEU
1	A	73	VAL
1	A	76	SER
1	A	83	THR
1	A	86	HIS
1	A	93	LYS
1	A	110	LEU

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Mol	Chain	Res	Type
1	A	120	LYS
1	A	121	ASP
1	A	134	LEU
1	A	136	ASN
1	A	144	GLN
1	A	145	LEU
1	A	146	LEU
1	A	147	SER
1	A	153	SER
1	A	155	GLU
1	A	156	THR
1	A	158	THR
1	A	162	ASN
1	A	165	LYS
1	A	167	MET
1	A	169	ASN
1	A	172	LEU
1	A	174	VAL
1	A	180	ASN
1	A	184	THR
1	A	185	LYS
1	A	186	SER
1	A	187	LYS
1	A	200	ASP
1	A	207	ASP
1	A	209	MET
1	A	232	ARG
1	A	240	ILE
1	A	259	THR
1	A	266	LYS
1	A	282	LEU
1	A	288	GLN
1	A	304	GLU
1	A	308	LYS
1	A	315	VAL
1	A	321	LYS
1	A	326	ARG
1	A	334	ARG
1	A	337	LEU
1	A	343	LEU
1	A	371	LEU
1	A	382	VAL

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Mol	Chain	Res	Type
1	A	388	LYS
1	A	390	ASP
1	A	398	LEU
1	A	402	ASN
1	A	408	LEU
1	A	410	GLU
1	B	2	ASP
1	B	3	LYS
1	B	4	LEU
1	B	7	LYS
1	B	11	ILE
1	B	13	LEU
1	B	33	ARG
1	B	39	SER
1	B	41	SER
1	B	53	LEU
1	B	83	THR
1	B	86	HIS
1	B	93	LYS
1	B	110	LEU
1	B	120	LYS
1	B	121	ASP
1	B	134	LEU
1	B	136	ASN
1	B	144	GLN
1	B	145	LEU
1	B	146	LEU
1	B	147	SER
1	B	150	ARG
1	B	153	SER
1	B	155	GLU
1	B	156	THR
1	B	162	ASN
1	B	165	LYS
1	B	167	MET
1	B	169	ASN
1	B	172	LEU
1	B	174	VAL
1	B	180	ASN
1	B	182	SER
1	B	185	LYS
1	B	186	SER

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Mol	Chain	Res	Type
1	B	187	LYS
1	B	200	ASP
1	B	204	ARG
1	B	207	ASP
1	B	209	MET
1	B	232	ARG
1	B	240	ILE
1	B	259	THR
1	B	266	LYS
1	B	282	LEU
1	B	288	GLN
1	B	304	GLU
1	B	308	LYS
1	B	315	VAL
1	B	321	LYS
1	B	326	ARG
1	B	334	ARG
1	B	337	LEU
1	B	342	ARG
1	B	343	LEU
1	B	371	LEU
1	B	382	VAL
1	B	385	LEU
1	B	387	LYS
1	B	388	LYS
1	B	390	ASP
1	B	398	LEU
1	B	402	ASN
1	B	408	LEU
1	B	410	GLU
1	C	2	ASP
1	C	3	LYS
1	C	4	LEU
1	C	7	LYS
1	C	13	LEU
1	C	27	GLU
1	C	33	ARG
1	C	39	SER
1	C	41	SER
1	C	53	LEU
1	C	73	VAL
1	C	83	THR

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Mol	Chain	Res	Type
1	C	86	HIS
1	C	93	LYS
1	C	110	LEU
1	C	120	LYS
1	C	121	ASP
1	C	134	LEU
1	C	136	ASN
1	C	144	GLN
1	C	145	LEU
1	C	146	LEU
1	C	147	SER
1	C	150	ARG
1	C	153	SER
1	C	155	GLU
1	C	156	THR
1	C	162	ASN
1	C	165	LYS
1	C	167	MET
1	C	169	ASN
1	C	172	LEU
1	C	174	VAL
1	C	180	ASN
1	C	185	LYS
1	C	186	SER
1	C	187	LYS
1	C	200	ASP
1	C	207	ASP
1	C	209	MET
1	C	232	ARG
1	C	240	ILE
1	C	259	THR
1	C	266	LYS
1	C	282	LEU
1	C	288	GLN
1	C	304	GLU
1	C	308	LYS
1	C	315	VAL
1	C	321	LYS
1	C	326	ARG
1	C	334	ARG
1	C	337	LEU
1	C	343	LEU

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Mol	Chain	Res	Type
1	C	371	LEU
1	C	382	VAL
1	C	387	LYS
1	C	388	LYS
1	C	390	ASP
1	C	398	LEU
1	C	402	ASN
1	C	408	LEU
1	C	410	GLU
1	D	2	ASP
1	D	3	LYS
1	D	4	LEU
1	D	7	LYS
1	D	11	ILE
1	D	13	LEU
1	D	33	ARG
1	D	37	MET
1	D	39	SER
1	D	41	SER
1	D	53	LEU
1	D	73	VAL
1	D	83	THR
1	D	86	HIS
1	D	93	LYS
1	D	110	LEU
1	D	120	LYS
1	D	121	ASP
1	D	134	LEU
1	D	140	THR
1	D	141	LYS
1	D	144	GLN
1	D	145	LEU
1	D	146	LEU
1	D	147	SER
1	D	153	SER
1	D	155	GLU
1	D	156	THR
1	D	158	THR
1	D	162	ASN
1	D	165	LYS
1	D	167	MET
1	D	169	ASN

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Mol	Chain	Res	Type
1	D	172	LEU
1	D	174	VAL
1	D	180	ASN
1	D	182	SER
1	D	185	LYS
1	D	186	SER
1	D	200	ASP
1	D	204	ARG
1	D	207	ASP
1	D	209	MET
1	D	232	ARG
1	D	240	ILE
1	D	243	ILE
1	D	259	THR
1	D	266	LYS
1	D	282	LEU
1	D	288	GLN
1	D	304	GLU
1	D	308	LYS
1	D	315	VAL
1	D	321	LYS
1	D	326	ARG
1	D	334	ARG
1	D	337	LEU
1	D	343	LEU
1	D	359	ASN
1	D	371	LEU
1	D	382	VAL
1	D	385	LEU
1	D	387	LYS
1	D	388	LYS
1	D	390	ASP
1	D	398	LEU
1	D	402	ASN
1	D	408	LEU
1	D	410	GLU
1	E	4	LEU
1	E	7	LYS
1	E	13	LEU
1	E	26	ASN
1	E	33	ARG
1	E	39	SER

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Mol	Chain	Res	Type
1	E	45	LYS
1	E	53	LEU
1	E	55	MET
1	E	86	HIS
1	E	93	LYS
1	E	110	LEU
1	E	116	THR
1	E	120	LYS
1	E	121	ASP
1	E	124	LEU
1	E	134	LEU
1	E	135	THR
1	E	140	THR
1	E	144	GLN
1	E	146	LEU
1	E	150	ARG
1	E	153	SER
1	E	154	GLU
1	E	155	GLU
1	E	157	THR
1	E	162	ASN
1	E	165	LYS
1	E	167	MET
1	E	172	LEU
1	E	174	VAL
1	E	185	LYS
1	E	186	SER
1	E	200	ASP
1	E	204	ARG
1	E	207	ASP
1	E	209	MET
1	E	241	THR
1	E	259	THR
1	E	266	LYS
1	E	281	ILE
1	E	282	LEU
1	E	288	GLN
1	E	304	GLU
1	E	308	LYS
1	E	315	VAL
1	E	321	LYS
1	E	326	ARG

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Mol	Chain	Res	Type
1	E	328	LEU
1	E	334	ARG
1	E	337	LEU
1	E	342	ARG
1	E	343	LEU
1	E	359	ASN
1	E	360	SER
1	E	370	GLU
1	E	371	LEU
1	E	382	VAL
1	E	385	LEU
1	E	387	LYS
1	E	388	LYS
1	E	390	ASP
1	E	398	LEU
1	E	402	ASN
1	E	407	LYS
1	E	408	LEU
1	E	409	THR
1	E	410	GLU
1	E	412	GLN
1	E	414	GLN
1	F	2	ASP
1	F	3	LYS
1	F	4	LEU
1	F	7	LYS
1	F	13	LEU
1	F	33	ARG
1	F	35	ARG
1	F	39	SER
1	F	41	SER
1	F	45	LYS
1	F	53	LEU
1	F	69	LEU
1	F	73	VAL
1	F	76	SER
1	F	84	GLN
1	F	96	ILE
1	F	120	LYS
1	F	121	ASP
1	F	134	LEU
1	F	135	THR

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Mol	Chain	Res	Type
1	F	140	THR
1	F	141	LYS
1	F	144	GLN
1	F	146	LEU
1	F	150	ARG
1	F	155	GLU
1	F	156	THR
1	F	157	THR
1	F	162	ASN
1	F	165	LYS
1	F	172	LEU
1	F	174	VAL
1	F	184	THR
1	F	185	LYS
1	F	197	SER
1	F	203	LYS
1	F	206	THR
1	F	207	ASP
1	F	209	MET
1	F	213	LYS
1	F	234	PHE
1	F	240	ILE
1	F	259	THR
1	F	272	VAL
1	F	278	VAL
1	F	280	ILE
1	F	282	LEU
1	F	284	ARG
1	F	288	GLN
1	F	292	ASP
1	F	297	ASN
1	F	304	GLU
1	F	308	LYS
1	F	326	ARG
1	F	330	LYS
1	F	337	LEU
1	F	342	ARG
1	F	344	VAL
1	F	371	LEU
1	F	382	VAL
1	F	385	LEU
1	F	387	LYS

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Mol	Chain	Res	Type
1	F	388	LYS
1	F	390	ASP
1	F	401	LEU
1	F	402	ASN
1	F	408	LEU
1	F	410	GLU
1	G	2	ASP
1	G	3	LYS
1	G	4	LEU
1	G	7	LYS
1	G	13	LEU
1	G	26	ASN
1	G	27	GLU
1	G	32	MET
1	G	33	ARG
1	G	37	MET
1	G	39	SER
1	G	41	SER
1	G	45	LYS
1	G	53	LEU
1	G	91	ILE
1	G	93	LYS
1	G	99	PHE
1	G	104	GLU
1	G	110	LEU
1	G	119	PHE
1	G	120	LYS
1	G	121	ASP
1	G	134	LEU
1	G	135	THR
1	G	136	ASN
1	G	141	LYS
1	G	144	GLN
1	G	146	LEU
1	G	147	SER
1	G	150	ARG
1	G	153	SER
1	G	155	GLU
1	G	156	THR
1	G	158	THR
1	G	160	VAL
1	G	162	ASN

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Mol	Chain	Res	Type
1	G	165	LYS
1	G	167	MET
1	G	172	LEU
1	G	185	LYS
1	G	186	SER
1	G	190	ASN
1	G	197	SER
1	G	200	ASP
1	G	207	ASP
1	G	209	MET
1	G	232	ARG
1	G	241	THR
1	G	242	GLU
1	G	259	THR
1	G	266	LYS
1	G	273	THR
1	G	279	ASP
1	G	282	LEU
1	G	290	LYS
1	G	295	VAL
1	G	297	ASN
1	G	304	GLU
1	G	308	LYS
1	G	321	LYS
1	G	326	ARG
1	G	334	ARG
1	G	337	LEU
1	G	342	ARG
1	G	371	LEU
1	G	382	VAL
1	G	385	LEU
1	G	387	LYS
1	G	388	LYS
1	G	390	ASP
1	G	395	GLU
1	G	397	HIS
1	G	402	ASN
1	G	410	GLU
1	G	418	MET
1	G	430	ARG
1	H	3	LYS
1	H	4	LEU

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Mol	Chain	Res	Type
1	H	7	LYS
1	H	18	ARG
1	H	21	LEU
1	H	26	ASN
1	H	33	ARG
1	H	34	MET
1	H	36	GLU
1	H	39	SER
1	H	41	SER
1	H	44	LEU
1	H	53	LEU
1	H	62	LEU
1	H	65	THR
1	H	84	GLN
1	H	86	HIS
1	H	93	LYS
1	H	104	GLU
1	H	110	LEU
1	H	116	THR
1	H	119	PHE
1	H	120	LYS
1	H	121	ASP
1	H	134	LEU
1	H	135	THR
1	H	138	ILE
1	H	139	HIS
1	H	140	THR
1	H	141	LYS
1	H	142	HIS
1	H	144	GLN
1	H	147	SER
1	H	153	SER
1	H	154	GLU
1	H	155	GLU
1	H	157	THR
1	H	162	ASN
1	H	163	LEU
1	H	165	LYS
1	H	169	ASN
1	H	172	LEU
1	H	173	LYS
1	H	174	VAL

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Mol	Chain	Res	Type
1	H	177	ILE
1	H	182	SER
1	H	185	LYS
1	H	186	SER
1	H	196	GLU
1	H	199	ILE
1	H	204	ARG
1	H	207	ASP
1	H	232	ARG
1	H	240	ILE
1	H	259	THR
1	H	277	CYS
1	H	279	ASP
1	H	281	ILE
1	H	282	LEU
1	H	284	ARG
1	H	288	GLN
1	H	295	VAL
1	H	297	ASN
1	H	304	GLU
1	H	308	LYS
1	H	315	VAL
1	H	321	LYS
1	H	325	ASP
1	H	326	ARG
1	H	330	LYS
1	H	334	ARG
1	H	342	ARG
1	H	343	LEU
1	H	356	VAL
1	H	362	THR
1	H	364	GLN
1	H	371	LEU
1	H	377	LYS
1	H	382	VAL
1	H	388	LYS
1	H	390	ASP
1	H	398	LEU
1	H	402	ASN
1	H	409	THR
1	H	418	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	84	GLN
1	A	136	ASN
1	A	144	GLN
1	A	247	ASN
1	A	250	GLN
1	A	269	ASN
1	A	313	ASN
1	A	352	HIS
1	A	383	HIS
1	A	412	GLN
1	A	414	GLN
1	B	26	ASN
1	B	84	GLN
1	B	136	ASN
1	B	144	GLN
1	B	247	ASN
1	B	250	GLN
1	B	269	ASN
1	B	288	GLN
1	B	313	ASN
1	B	383	HIS
1	B	412	GLN
1	B	414	GLN
1	C	26	ASN
1	C	84	GLN
1	C	136	ASN
1	C	144	GLN
1	C	247	ASN
1	C	250	GLN
1	C	269	ASN
1	C	313	ASN
1	C	352	HIS
1	C	364	GLN
1	C	383	HIS
1	C	412	GLN
1	C	414	GLN
1	D	26	ASN
1	D	84	GLN
1	D	136	ASN
1	D	144	GLN
1	D	247	ASN

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Mol	Chain	Res	Type
1	D	250	GLN
1	D	269	ASN
1	D	383	HIS
1	D	412	GLN
1	D	414	GLN
1	E	26	ASN
1	E	84	GLN
1	E	115	GLN
1	E	136	ASN
1	E	144	GLN
1	E	229	GLN
1	E	247	ASN
1	E	269	ASN
1	E	288	GLN
1	E	319	ASN
1	E	333	HIS
1	E	352	HIS
1	E	364	GLN
1	E	383	HIS
1	E	412	GLN
1	E	414	GLN
1	F	26	ASN
1	F	84	GLN
1	F	136	ASN
1	F	247	ASN
1	F	250	GLN
1	F	313	ASN
1	F	319	ASN
1	F	383	HIS
1	F	412	GLN
1	F	414	GLN
1	G	26	ASN
1	G	84	GLN
1	G	136	ASN
1	G	144	GLN
1	G	250	GLN
1	G	269	ASN
1	G	300	HIS
1	G	319	ASN
1	G	363	ASN
1	G	364	GLN
1	G	368	GLN

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Mol	Chain	Res	Type
1	G	414	GLN
1	H	26	ASN
1	H	115	GLN
1	H	136	ASN
1	H	144	GLN
1	H	247	ASN
1	H	250	GLN
1	H	269	ASN
1	H	288	GLN
1	H	352	HIS
1	H	364	GLN
1	H	383	HIS
1	H	412	GLN
1	H	414	GLN
1	H	428	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	A	1432	-	38,48,48	2.11	8 (21%)	47,73,73	1.69	6 (12%)
3	DEA	A	1433	-	13,19,19	0.95	0	8,27,27	0.93	0
2	NAD	B	2432	-	38,48,48	2.02	7 (18%)	47,73,73	1.71	8 (17%)
3	DEA	B	2433	-	13,19,19	1.00	0	8,27,27	0.90	0
2	NAD	C	3432	-	38,48,48	2.09	8 (21%)	47,73,73	1.66	7 (14%)
3	DEA	C	3433	-	13,19,19	0.90	0	8,27,27	0.93	0
2	NAD	D	4432	-	38,48,48	2.13	6 (15%)	47,73,73	1.70	9 (19%)
3	DEA	D	4433	-	13,19,19	1.21	2 (15%)	8,27,27	0.93	0
2	NAD	E	5432	-	38,48,48	2.01	6 (15%)	47,73,73	1.65	6 (12%)
3	DEA	E	5433	-	13,19,19	0.87	0	8,27,27	1.01	0
2	NAD	F	6432	-	38,48,48	2.10	8 (21%)	47,73,73	1.65	8 (17%)
3	DEA	F	6433	-	13,19,19	0.97	0	8,27,27	1.11	1 (12%)
2	NAD	G	7432	-	38,48,48	2.12	7 (18%)	47,73,73	1.68	6 (12%)
3	DEA	G	7433	-	13,19,19	1.19	1 (7%)	8,27,27	0.98	0
2	NAD	H	8432	-	38,48,48	2.00	5 (13%)	47,73,73	1.71	8 (17%)
3	DEA	H	8433	-	13,19,19	0.95	0	8,27,27	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	1432	-	-	0/22/62/62	0/5/5/5
3	DEA	A	1433	-	-	0/6/12/12	0/2/2/2
2	NAD	B	2432	-	-	0/22/62/62	0/5/5/5
3	DEA	B	2433	-	-	0/6/12/12	0/2/2/2
2	NAD	C	3432	-	-	0/22/62/62	0/5/5/5
3	DEA	C	3433	-	-	0/6/12/12	0/2/2/2
2	NAD	D	4432	-	-	0/22/62/62	0/5/5/5
3	DEA	D	4433	-	-	0/6/12/12	0/2/2/2
2	NAD	E	5432	-	-	0/22/62/62	0/5/5/5
3	DEA	E	5433	-	-	0/6/12/12	0/2/2/2
2	NAD	F	6432	-	-	0/22/62/62	0/5/5/5
3	DEA	F	6433	-	-	0/6/12/12	0/2/2/2
2	NAD	G	7432	-	-	0/22/62/62	0/5/5/5
3	DEA	G	7433	-	-	0/6/12/12	0/2/2/2
2	NAD	H	8432	-	-	0/22/62/62	0/5/5/5
3	DEA	H	8433	-	-	0/6/12/12	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5432	NAD	O4B-C1B	-4.76	1.35	1.41
2	G	7432	NAD	O4B-C1B	-4.62	1.35	1.41
2	F	6432	NAD	O4B-C1B	-4.38	1.35	1.41
2	C	3432	NAD	O4B-C1B	-4.20	1.35	1.41
2	A	1432	NAD	O4B-C1B	-4.19	1.35	1.41
2	B	2432	NAD	O4B-C1B	-3.99	1.36	1.41
2	D	4432	NAD	O4B-C1B	-3.58	1.36	1.41
2	H	8432	NAD	O4B-C1B	-3.18	1.37	1.41
2	F	6432	NAD	C6N-C5N	-2.22	1.33	1.38
2	A	1432	NAD	C6N-C5N	-2.18	1.33	1.38
2	C	3432	NAD	C6N-C5N	-2.15	1.33	1.38
2	G	7432	NAD	C6N-C5N	-2.11	1.33	1.38
2	E	5432	NAD	C2A-N1A	2.13	1.37	1.33
3	G	7433	DEA	C2'-C3'	2.17	1.55	1.53
2	C	3432	NAD	C7N-N7N	2.17	1.37	1.33
3	D	4433	DEA	C2'-C3'	2.18	1.55	1.53
2	B	2432	NAD	C2A-N1A	2.18	1.38	1.33
2	B	2432	NAD	C7N-N7N	2.19	1.37	1.33
2	C	3432	NAD	C2A-N1A	2.27	1.38	1.33
3	D	4433	DEA	C2-N3	2.36	1.36	1.32
2	F	6432	NAD	C7N-N7N	2.37	1.37	1.33
2	A	1432	NAD	C7N-N7N	2.37	1.37	1.33
2	G	7432	NAD	C2A-N1A	2.40	1.38	1.33
2	A	1432	NAD	C2A-N1A	2.44	1.38	1.33
2	F	6432	NAD	C2A-N1A	2.46	1.38	1.33
2	D	4432	NAD	C2A-N1A	2.58	1.38	1.33
2	H	8432	NAD	C6N-N1N	3.23	1.44	1.35
2	B	2432	NAD	C6N-N1N	3.43	1.44	1.35
2	F	6432	NAD	C6N-N1N	3.48	1.44	1.35
2	E	5432	NAD	C6N-N1N	3.50	1.44	1.35
2	A	1432	NAD	C6N-N1N	3.56	1.45	1.35
2	G	7432	NAD	C6N-N1N	3.65	1.45	1.35
2	D	4432	NAD	C6N-N1N	3.70	1.45	1.35
2	C	3432	NAD	C6N-N1N	3.74	1.45	1.35
2	F	6432	NAD	C2N-C3N	5.11	1.46	1.39
2	E	5432	NAD	C2N-C3N	5.14	1.46	1.39
2	H	8432	NAD	C4N-C3N	5.30	1.48	1.39
2	E	5432	NAD	C4N-C3N	5.45	1.48	1.39
2	A	1432	NAD	C2N-C3N	5.53	1.47	1.39
2	B	2432	NAD	C4N-C3N	5.54	1.48	1.39
2	C	3432	NAD	C4N-C3N	5.58	1.48	1.39
2	B	2432	NAD	C2N-C3N	5.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7432	NAD	C4N-C3N	5.80	1.49	1.39
2	C	3432	NAD	C2N-C3N	5.87	1.47	1.39
2	F	6432	NAD	C4N-C3N	5.88	1.49	1.39
2	D	4432	NAD	C4N-C3N	5.89	1.49	1.39
2	H	8432	NAD	C2N-C3N	5.94	1.48	1.39
2	A	1432	NAD	C4N-C3N	5.94	1.49	1.39
2	G	7432	NAD	C2N-C3N	6.07	1.48	1.39
2	D	4432	NAD	C2N-C3N	6.23	1.48	1.39
2	C	3432	NAD	C5N-C4N	6.41	1.52	1.38
2	G	7432	NAD	C5N-C4N	6.43	1.52	1.38
2	E	5432	NAD	C5N-C4N	6.45	1.52	1.38
2	B	2432	NAD	C5N-C4N	6.48	1.52	1.38
2	H	8432	NAD	C5N-C4N	6.63	1.52	1.38
2	A	1432	NAD	C5N-C4N	6.64	1.52	1.38
2	F	6432	NAD	C5N-C4N	6.65	1.52	1.38
2	D	4432	NAD	C5N-C4N	6.83	1.53	1.38

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	7432	NAD	O7N-C7N-C3N	-6.15	112.88	119.59
2	A	1432	NAD	O7N-C7N-C3N	-5.95	113.09	119.59
2	D	4432	NAD	O7N-C7N-C3N	-5.92	113.13	119.59
2	B	2432	NAD	O7N-C7N-C3N	-5.91	113.13	119.59
2	C	3432	NAD	O7N-C7N-C3N	-5.89	113.16	119.59
2	H	8432	NAD	O7N-C7N-C3N	-5.78	113.28	119.59
2	F	6432	NAD	O7N-C7N-C3N	-5.77	113.28	119.59
2	E	5432	NAD	O7N-C7N-C3N	-5.69	113.38	119.59
2	D	4432	NAD	C5N-C4N-C3N	-3.29	116.19	120.33
2	H	8432	NAD	C5N-C4N-C3N	-3.26	116.23	120.33
2	B	2432	NAD	C5N-C4N-C3N	-3.25	116.25	120.33
2	E	5432	NAD	C5N-C4N-C3N	-3.24	116.26	120.33
2	G	7432	NAD	C5N-C4N-C3N	-3.14	116.39	120.33
2	F	6432	NAD	C5N-C4N-C3N	-3.10	116.44	120.33
2	A	1432	NAD	C5N-C4N-C3N	-3.06	116.49	120.33
2	C	3432	NAD	C5N-C4N-C3N	-3.03	116.52	120.33
2	H	8432	NAD	PN-O3-PA	-2.88	124.64	132.73
2	F	6432	NAD	O3-PN-O5D	-2.49	96.33	102.94
2	B	2432	NAD	O3-PN-O5D	-2.46	96.41	102.94
2	C	3432	NAD	PN-O3-PA	-2.33	126.19	132.73
2	E	5432	NAD	O3-PN-O5D	-2.30	96.83	102.94
2	D	4432	NAD	N3A-C2A-N1A	-2.25	127.17	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4432	NAD	O3-PN-O5D	-2.24	96.99	102.94
2	H	8432	NAD	O3-PN-O5D	-2.22	97.06	102.94
2	A	1432	NAD	O5B-C5B-C4B	-2.14	101.24	109.12
2	B	2432	NAD	PN-O3-PA	-2.14	126.73	132.73
2	F	6432	NAD	O5B-C5B-C4B	-2.12	101.29	109.12
2	D	4432	NAD	O5B-C5B-C4B	-2.09	101.41	109.12
2	C	3432	NAD	O5B-C5B-C4B	-2.04	101.58	109.12
3	F	6433	DEA	N3-C2-N1	-2.01	127.36	128.89
2	G	7432	NAD	O3-PN-O5D	-2.00	97.63	102.94
2	B	2432	NAD	O3-PA-O5B	2.01	108.26	102.94
2	D	4432	NAD	O3-PA-O5B	2.07	108.42	102.94
2	F	6432	NAD	C4A-C5A-N7A	2.11	111.42	109.48
2	F	6432	NAD	C5N-C6N-N1N	2.13	124.16	120.47
2	B	2432	NAD	C5N-C6N-N1N	2.24	124.34	120.47
2	D	4432	NAD	C5N-C6N-N1N	2.26	124.38	120.47
2	G	7432	NAD	C4A-C5A-N7A	2.26	111.56	109.48
2	H	8432	NAD	C5N-C6N-N1N	2.27	124.39	120.47
2	F	6432	NAD	O3-PA-O5B	2.27	108.97	102.94
2	A	1432	NAD	C5N-C6N-N1N	2.28	124.42	120.47
2	E	5432	NAD	C5N-C6N-N1N	2.29	124.43	120.47
2	H	8432	NAD	O3-PA-O5B	2.34	109.15	102.94
2	C	3432	NAD	C5N-C6N-N1N	2.38	124.60	120.47
2	E	5432	NAD	C4A-C5A-N7A	2.44	111.73	109.48
2	B	2432	NAD	C4A-C5A-N7A	2.45	111.73	109.48
2	C	3432	NAD	C4A-C5A-N7A	2.47	111.75	109.48
2	D	4432	NAD	C4A-C5A-N7A	2.48	111.76	109.48
2	G	7432	NAD	C5N-C6N-N1N	2.50	124.80	120.47
2	A	1432	NAD	C4A-C5A-N7A	2.52	111.80	109.48
2	H	8432	NAD	C4A-C5A-N7A	2.62	111.89	109.48
2	E	5432	NAD	C3N-C7N-N7N	5.80	124.17	117.82
2	F	6432	NAD	C3N-C7N-N7N	6.07	124.46	117.82
2	C	3432	NAD	C3N-C7N-N7N	6.16	124.56	117.82
2	H	8432	NAD	C3N-C7N-N7N	6.23	124.63	117.82
2	A	1432	NAD	C3N-C7N-N7N	6.28	124.69	117.82
2	D	4432	NAD	C3N-C7N-N7N	6.37	124.79	117.82
2	B	2432	NAD	C3N-C7N-N7N	6.39	124.81	117.82
2	G	7432	NAD	C3N-C7N-N7N	6.49	124.92	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1432	NAD	2	0
2	B	2432	NAD	3	0
2	C	3432	NAD	3	0
2	D	4432	NAD	2	0
2	E	5432	NAD	3	0
2	F	6432	NAD	2	0
3	F	6433	DEA	1	0
2	G	7432	NAD	6	0
2	H	8432	NAD	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	430/431 (99%)	-0.35	1 (0%)	95	87	2, 3, 4, 6	0
1	B	430/431 (99%)	-0.26	2 (0%)	91	76	2, 3, 4, 7	0
1	C	430/431 (99%)	-0.32	1 (0%)	95	87	2, 3, 4, 6	0
1	D	430/431 (99%)	-0.32	1 (0%)	95	87	2, 3, 4, 7	0
1	E	430/431 (99%)	-0.42	1 (0%)	95	87	2, 2, 4, 5	0
1	F	430/431 (99%)	-0.42	2 (0%)	91	76	2, 2, 4, 7	0
1	G	430/431 (99%)	-0.41	1 (0%)	95	87	2, 2, 4, 6	0
1	H	430/431 (99%)	-0.41	1 (0%)	95	87	2, 2, 4, 7	0
All	All	3440/3448 (99%)	-0.36	10 (0%)	94	84	2, 2, 4, 7	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ASP	3.7
1	H	2	ASP	3.5
1	A	2	ASP	3.3
1	B	2	ASP	3.2
1	F	2	ASP	3.0
1	G	2	ASP	2.9
1	E	2	ASP	2.9
1	C	3	LYS	2.6
1	B	376	ASP	2.1
1	F	3	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	DEA	H	8433	18/18	0.91	0.21	1.80	2,2,3,3	0
3	DEA	G	7433	18/18	0.90	0.22	1.31	2,2,5,6	0
3	DEA	C	3433	18/18	0.89	0.24	0.96	2,2,5,5	0
3	DEA	B	2433	18/18	0.89	0.21	0.82	2,2,4,5	0
3	DEA	A	1433	18/18	0.92	0.21	0.79	2,2,4,5	0
3	DEA	E	5433	18/18	0.94	0.19	0.46	2,2,3,3	0
3	DEA	D	4433	18/18	0.91	0.20	0.05	2,2,3,4	0
3	DEA	F	6433	18/18	0.91	0.18	0.02	2,2,4,4	0
2	NAD	H	8432	44/44	0.95	0.17	-0.23	2,2,4,5	0
2	NAD	A	1432	44/44	0.94	0.18	-0.24	2,2,3,4	0
2	NAD	C	3432	44/44	0.95	0.18	-0.31	2,2,3,3	0
2	NAD	B	2432	44/44	0.95	0.17	-0.32	2,2,3,4	0
2	NAD	F	6432	44/44	0.96	0.16	-0.73	2,2,3,4	0
2	NAD	E	5432	44/44	0.95	0.16	-0.80	2,2,3,4	0
2	NAD	G	7432	44/44	0.95	0.15	-1.03	2,2,3,3	0
2	NAD	D	4432	44/44	0.95	0.14	-1.10	2,2,3,3	0

6.5 Other polymers (i)

There are no such residues in this entry.