



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:33 am GMT

PDB ID : 3RVD  
Title : Crystal structure of the binary complex, obtained by soaking, of photosynthetic a4 glyceraldehyde 3-phosphate dehydrogenase (gapdh) with cp12-2, both from arabidopsis thaliana.  
Authors : Fermani, S.; Thumiger, A.; Falini, G.; Marri, L.; Sparla, F.; Trost, P.  
Deposited on : 2011-05-06  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28683
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

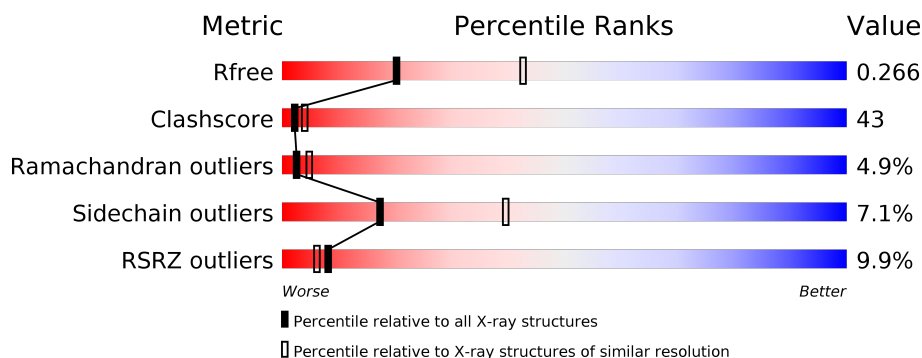
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



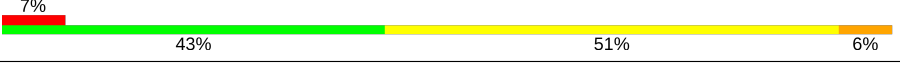





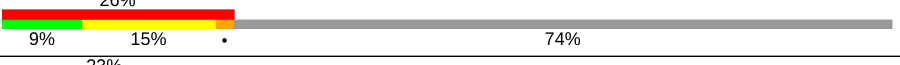



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	<div> <div>51%</div> <div>44%</div> <div>5%</div> </div>
1	B	337	<div> <div>3%</div> <div>46%</div> <div>47%</div> <div>7%</div> </div>
1	C	337	<div> <div>4%</div> <div>51%</div> <div>42%</div> <div>7%</div> </div>
1	D	337	<div> <div>7%</div> <div>30%</div> <div>58%</div> <div>11%</div> </div>
1	E	337	<div> <div>36%</div> <div>25%</div> <div>64%</div> <div>10%</div> </div>
1	F	337	<div> <div>18%</div> <div>28%</div> <div>62%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	337	
1	H	337	
1	O	337	
1	Q	337	
2	I	82	
2	J	82	
2	K	82	
2	L	82	
2	M	82	
2	N	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	407	-	-	-	X
4	SO4	B	403	-	-	-	X
4	SO4	C	406	-	-	-	X
4	SO4	O	402	-	-	-	X
4	SO4	O	403	-	-	-	X
4	SO4	Q	403	-	-	-	X
4	SO4	Q	404	-	-	-	X
4	SO4	Q	405	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27674 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 Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	B	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	C	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	D	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	E	336	Total	C	N	O	S	0	0	0
			2547	1609	443	486	9			
1	F	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			
1	G	337	Total	C	N	O	S	0	0	0
			2556	1615	445	487	9			
1	H	335	Total	C	N	O	S	0	0	0
			2542	1606	442	485	9			
1	O	337	Total	C	N	O	S	0	0	0
			2557	1615	445	488	9			
1	Q	336	Total	C	N	O	S	0	0	0
			2552	1612	444	487	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	EXPRESSION TAG	UNP P25856
B	-1	ALA	-	EXPRESSION TAG	UNP P25856
C	-1	ALA	-	EXPRESSION TAG	UNP P25856
D	-1	ALA	-	EXPRESSION TAG	UNP P25856
E	-1	ALA	-	EXPRESSION TAG	UNP P25856
F	-1	ALA	-	EXPRESSION TAG	UNP P25856
G	-1	ALA	-	EXPRESSION TAG	UNP P25856
H	-1	ALA	-	EXPRESSION TAG	UNP P25856
O	-1	ALA	-	EXPRESSION TAG	UNP P25856

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-1	ALA	-	EXPRESSION TAG	UNP P25856

- Molecule 2 is a protein called Photosynthetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	22	Total	C	N	O	S	0	0	0
			182	107	29	44	2			
2	J	21	Total	C	N	O	S	0	0	0
			176	104	28	42	2			
2	K	21	Total	C	N	O	S	0	0	0
			176	104	28	42	2			
2	L	19	Total	C	N	O	S	0	0	0
			148	86	22	38	2			
2	M	22	Total	C	N	O	S	0	0	0
			182	107	29	44	2			
2	N	19	Total	C	N	O	S	0	0	0
			160	96	25	37	2			

There are 24 discrepancies between the modelled and reference sequences:

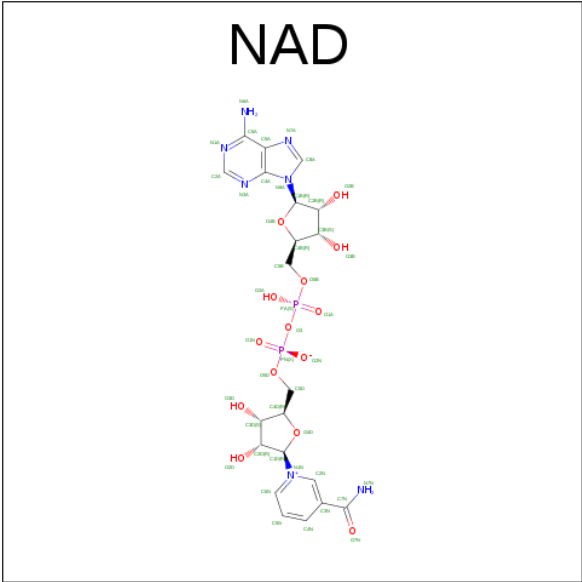
Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
I	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
I	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
I	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
J	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
J	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
J	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
J	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
K	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
K	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
K	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
K	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
L	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
L	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
L	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
L	0	MET	-	EXPRESSION TAG	UNP Q9LZP9
M	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
M	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
M	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
M	0	MET	-	EXPRESSION TAG	UNP Q9LZP9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	GLY	-	EXPRESSION TAG	UNP Q9LZP9
N	-2	SER	-	EXPRESSION TAG	UNP Q9LZP9
N	-1	HIS	-	EXPRESSION TAG	UNP Q9LZP9
N	0	MET	-	EXPRESSION TAG	UNP Q9LZP9

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



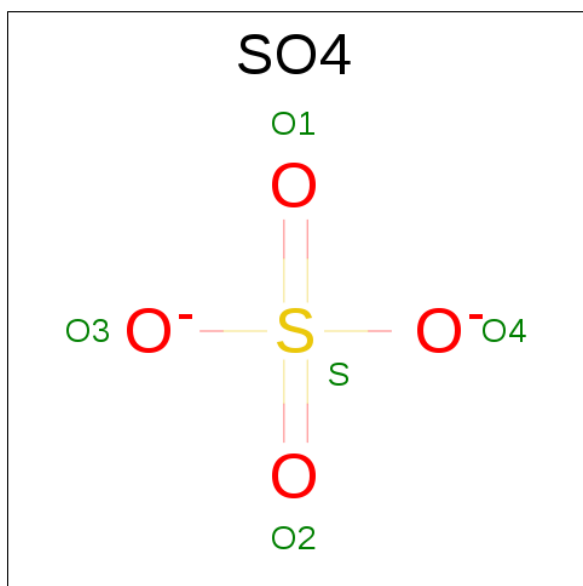
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	O	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		
4	Q	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		

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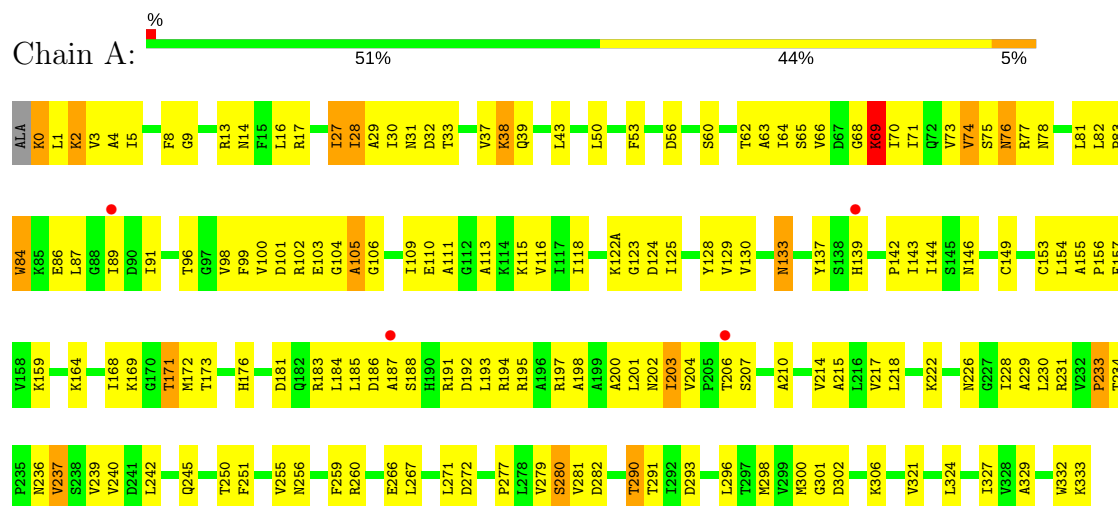
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	35	Total 35	O 35	0	0
5	C	55	Total 55	O 55	0	0
5	D	52	Total 52	O 52	0	0
5	E	42	Total 42	O 42	0	0
5	F	36	Total 36	O 36	0	0
5	G	38	Total 38	O 38	0	0
5	H	31	Total 31	O 31	0	0
5	I	3	Total 3	O 3	0	0
5	J	1	Total 1	O 1	0	0
5	K	20	Total 20	O 20	0	0
5	L	4	Total 4	O 4	0	0
5	M	6	Total 6	O 6	0	0
5	N	10	Total 10	O 10	0	0
5	O	82	Total 82	O 82	0	0
5	Q	69	Total 69	O 69	0	0

### 3 Residue-property plots

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

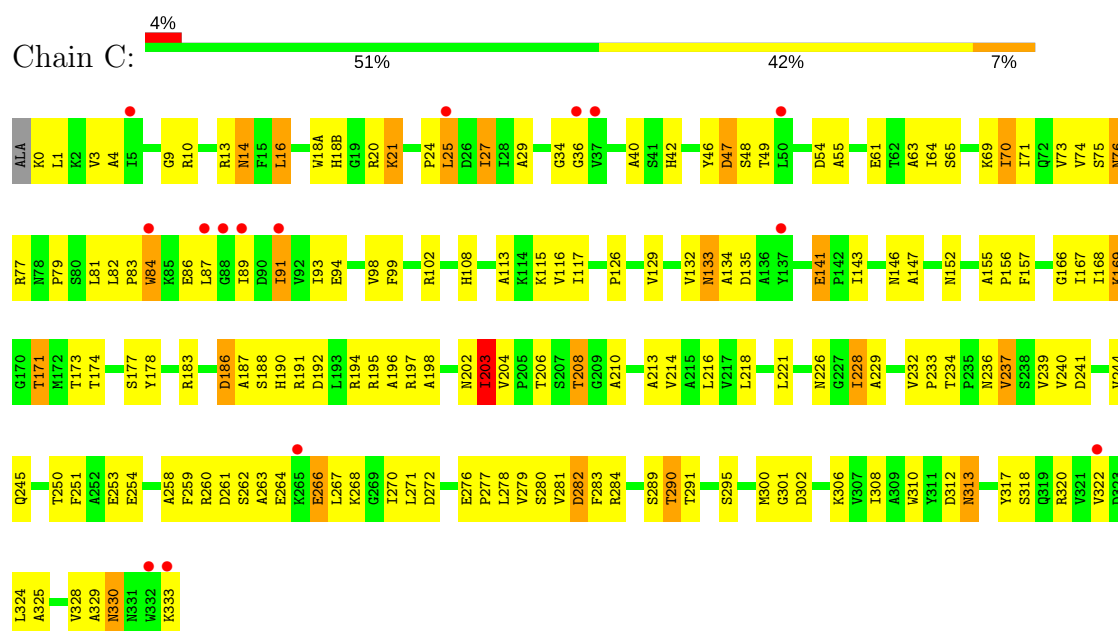
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



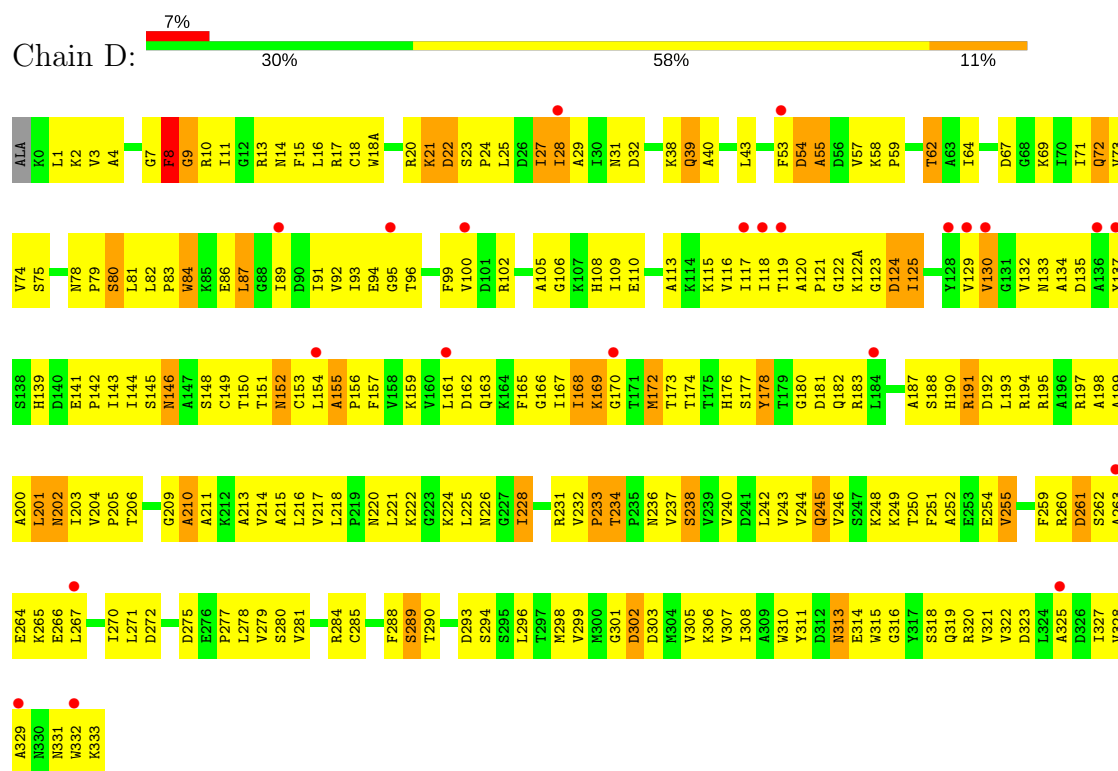
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic



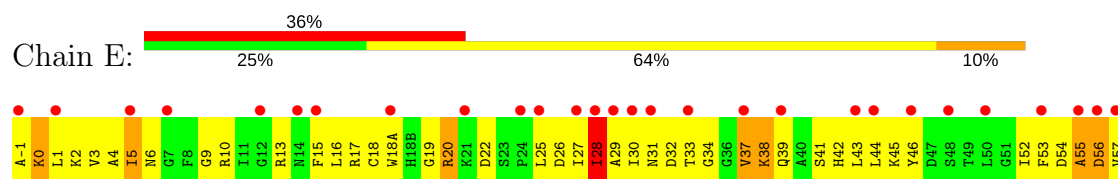
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

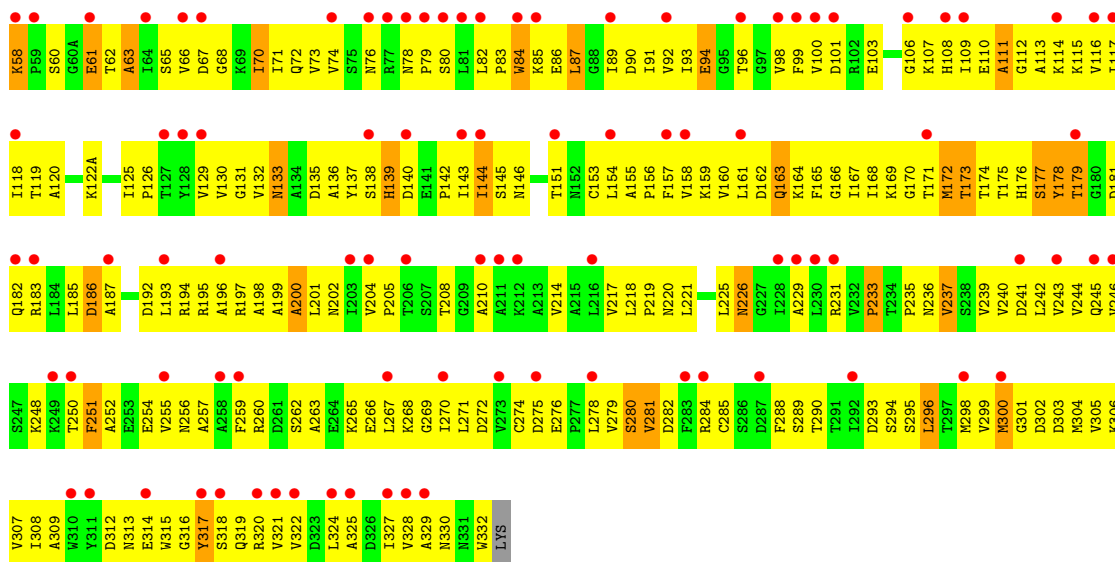


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

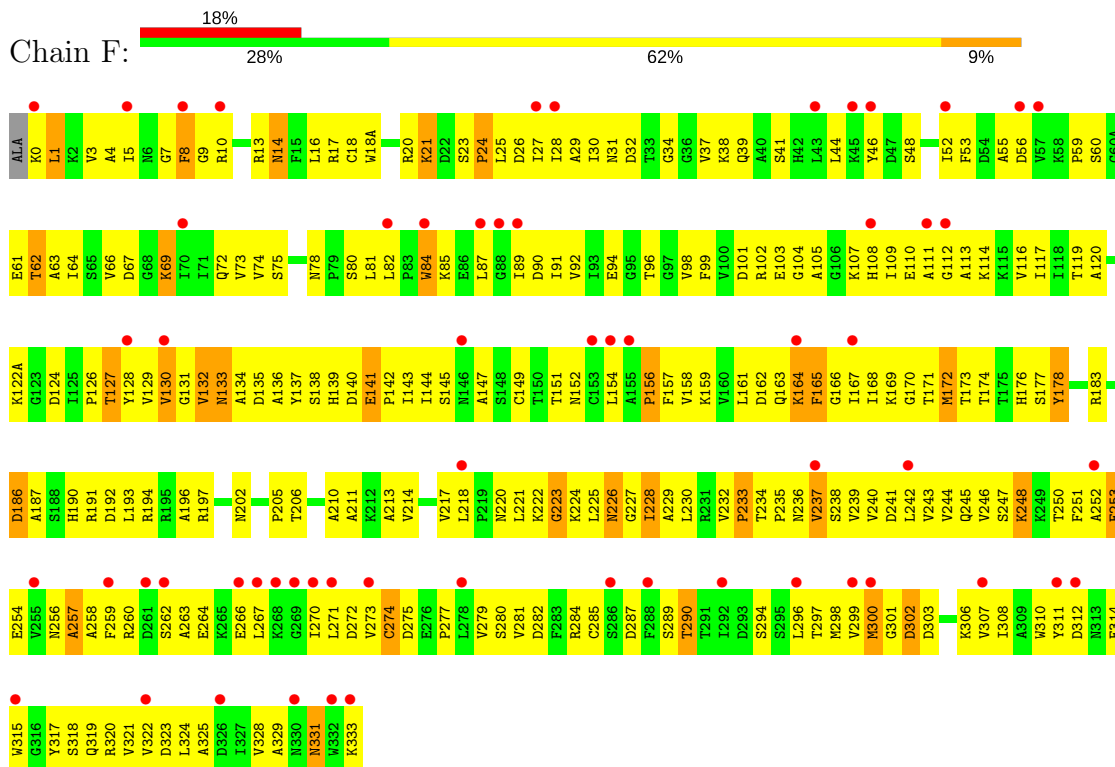


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

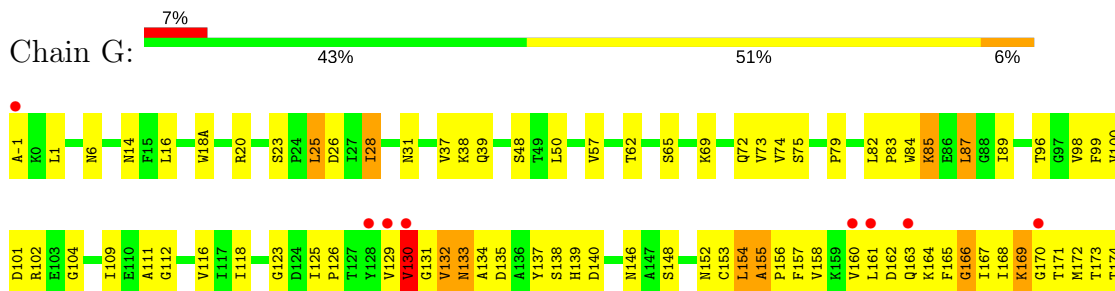


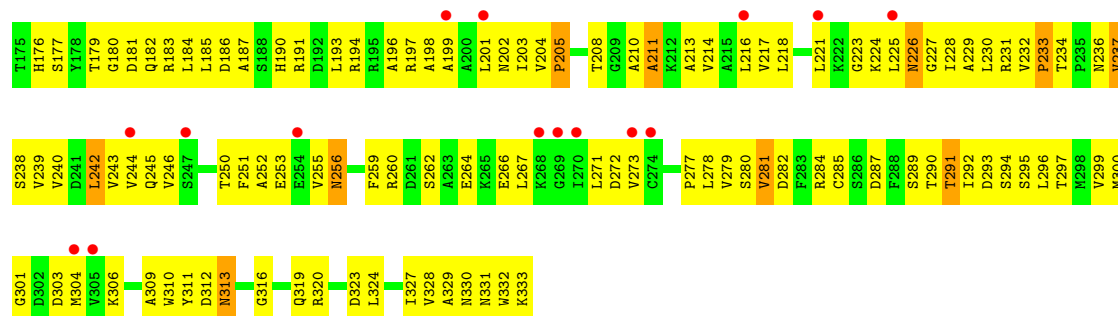


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

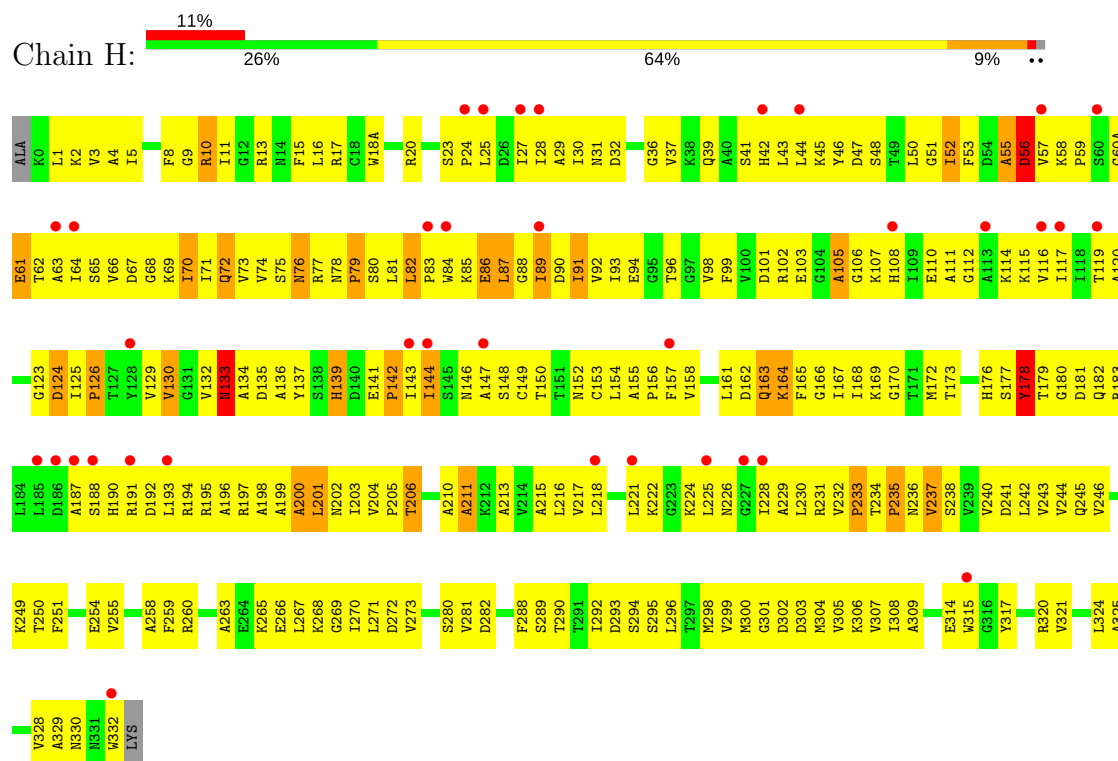


• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplatic

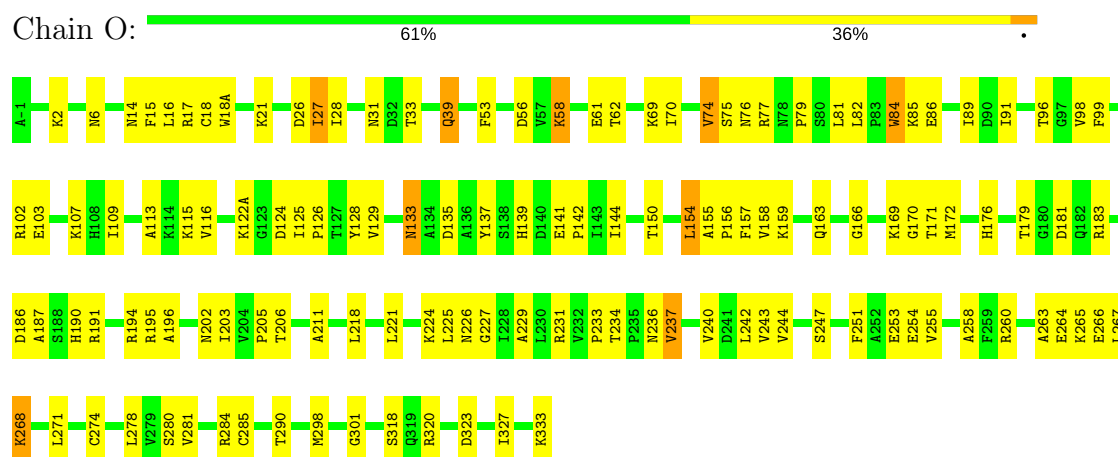




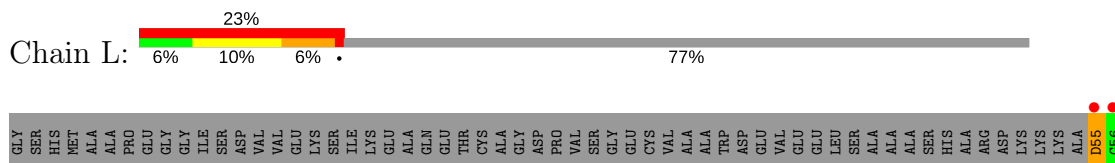
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

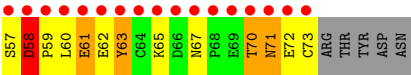


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

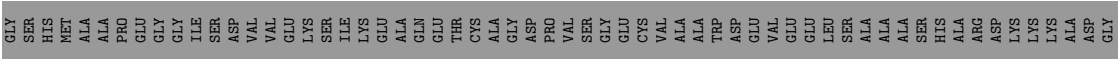


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A, chloroplastic

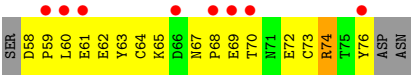




● Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)



● Molecule 2: Photosyntetic glyceraldehyde-3-phosphate dehydrogenase (a4 isoform)



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.18Å 188.75Å 312.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.61 – 2.70 94.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (94.61-2.70) 95.8 (94.60-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.247 , 0.318 0.243 , 0.266	Depositor DCC
$R_{free}$ test set	11850 reflections (10.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 86.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.45	0/2596	0.69	1/3523 (0.0%)
1	B	0.44	0/2596	0.73	2/3523 (0.1%)
1	C	0.44	0/2596	0.70	1/3523 (0.0%)
1	D	0.40	0/2596	0.66	0/3523
1	E	0.44	0/2591	0.68	0/3519
1	F	0.40	0/2596	0.64	0/3523
1	G	0.42	0/2600	0.68	0/3530
1	H	0.40	0/2586	0.65	0/3512
1	O	0.55	0/2601	0.77	1/3530 (0.0%)
1	Q	0.51	0/2596	0.77	2/3523 (0.1%)
2	I	0.75	0/185	0.64	0/251
2	J	0.84	1/179 (0.6%)	0.64	0/243
2	K	0.46	0/179	0.65	0/243
2	L	0.64	0/150	0.86	0/203
2	M	0.66	0/185	0.70	0/251
2	N	0.55	0/163	0.56	0/221
All	All	0.46	1/26995 (0.0%)	0.70	7/36641 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	61	GLU	CG-CD	5.06	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	203	ILE	N-CA-C	-6.16	94.37	111.00
1	O	203	ILE	N-CA-C	-5.87	95.16	111.00
1	B	203	ILE	N-CA-C	-5.82	95.30	111.00
1	A	203	ILE	N-CA-C	-5.62	95.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	60(A)	GLY	N-CA-C	-5.54	99.24	113.10
1	C	203	ILE	N-CA-C	-5.53	96.08	111.00
1	B	34	GLY	N-CA-C	5.52	126.89	113.10

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	2552	0	2593	200	0
1	B	2552	0	2593	218	0
1	C	2552	0	2593	198	0
1	D	2552	0	2593	318	0
1	E	2547	0	2585	369	0
1	F	2552	0	2593	312	0
1	G	2556	0	2598	264	0
1	H	2542	0	2580	338	0
1	O	2557	0	2598	135	0
1	Q	2552	0	2593	129	0
2	I	182	0	149	25	0
2	J	176	0	144	14	0
2	K	176	0	144	25	0
2	L	148	0	117	23	0
2	M	182	0	149	23	0
2	N	160	0	134	31	0
3	A	44	0	26	3	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	6	0
3	E	44	0	26	5	0
3	F	44	0	26	6	0
3	G	44	0	26	1	0
3	H	44	0	26	13	0
3	O	44	0	26	0	0
3	Q	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	0	1	0
4	B	10	0	0	1	0
4	C	25	0	0	1	0
4	D	5	0	0	1	0
4	E	15	0	0	2	0
4	F	10	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	O	10	0	0	0	0
4	Q	20	0	0	1	0
5	A	72	0	0	3	0
5	B	35	0	0	2	0
5	C	55	0	0	1	0
5	D	52	0	0	4	0
5	E	42	0	0	6	0
5	F	36	0	0	5	0
5	G	38	0	0	3	0
5	H	31	0	0	1	0
5	I	3	0	0	0	0
5	J	1	0	0	0	0
5	K	20	0	0	1	0
5	L	4	0	0	2	0
5	M	6	0	0	1	0
5	N	10	0	0	2	0
5	O	82	0	0	3	0
5	Q	69	0	0	3	1
All	All	27674	0	27016	2311	1

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 43.

All (2311) 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:D:117:ILE:HG23	1:D:144:ILE:HD11	1.23	1.17
1:D:78:ASN:HD22	1:D:81:LEU:HG	1.11	1.13
1:G:161:LEU:HB3	1:G:167:ILE:HD11	1.19	1.12
1:A:202:ASN:HD21	1:C:281:VAL:HG12	1.06	1.11
1:C:183:ARG:HE	1:C:187:ALA:HB3	1.12	1.11
1:B:208:THR:HG23	1:B:209:GLY:H	1.17	1.06
1:F:59:PRO:HA	1:F:64:ILE:HG22	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LYS:HD3	2:M:57:SER:HA	1.38	1.05
1:F:117:ILE:HA	1:F:144:ILE:HD11	1.35	1.04
1:E:194:ARG:HH21	1:G:277:PRO:HA	1.21	1.02
1:A:65:SER:HB3	1:A:70:ILE:HD13	1.38	1.01
1:H:2:LYS:HD2	1:H:88:GLY:HA2	1.40	1.01
1:B:139:HIS:HB3	1:B:333:LYS:HE2	1.41	1.01
1:D:299:VAL:HG22	1:D:305:VAL:HG22	1.41	1.00
1:E:169:LYS:HD2	1:G:301:GLY:HA3	1.44	1.00
1:F:176:HIS:HA	1:F:238:SER:HB3	1.43	1.00
1:G:271:LEU:HD11	1:G:292:ILE:HD13	1.45	0.99
1:E:262:SER:HB3	1:E:267:LEU:HD12	1.44	0.97
1:O:6:ASN:ND2	1:O:31:ASN:HD22	1.61	0.97
1:H:181:ASP:HB3	1:H:195:ARG:HD3	1.47	0.97
1:E:160:VAL:O	1:E:164:LYS:HB2	1.64	0.96
1:E:202:ASN:HB3	1:G:281:VAL:HG23	1.48	0.96
1:E:186:ASP:HB2	1:H:10:ARG:NH1	1.81	0.95
2:M:62:GLU:HG3	5:M:101:HOH:O	1.64	0.95
1:E:117:ILE:HG12	1:E:144:ILE:HD11	1.46	0.95
1:E:204:VAL:HB	1:E:231:ARG:HB2	1.46	0.94
1:G:221:LEU:HD11	1:G:225:LEU:HG	1.47	0.94
1:D:149:CYS:SG	2:I:78:ASN:ND2	2.42	0.93
1:F:318:SER:O	1:F:322:VAL:HG23	1.67	0.93
1:A:202:ASN:ND2	1:C:281:VAL:HG12	1.83	0.93
2:J:71:ASN:HA	2:J:74:ARG:HH21	1.31	0.92
2:K:69:GLU:HB3	1:O:98:VAL:HG11	1.49	0.92
1:F:202:ASN:HD22	1:H:281:VAL:HG23	1.33	0.91
1:H:215:ALA:HB1	1:H:222:LYS:HA	1.53	0.91
1:E:70:ILE:HD13	1:E:70:ILE:H	1.35	0.91
1:Q:331:ASN:HD22	1:Q:331:ASN:N	1.67	0.91
1:G:271:LEU:HD13	1:G:290:THR:HG23	1.54	0.90
1:D:78:ASN:HD21	1:D:80:SER:HB2	1.36	0.90
1:E:279:VAL:HG11	1:G:204:VAL:HG22	1.53	0.90
1:F:129:VAL:HG23	1:F:217:VAL:HG11	1.53	0.90
1:F:245:GLN:HE21	1:H:245:GLN:NE2	1.70	0.90
1:E:17:ARG:CZ	1:E:53:PHE:HB2	2.02	0.89
1:D:62:THR:OG1	1:H:74:VAL:HG13	1.70	0.89
1:B:233:PRO:HB2	1:D:233:PRO:HB2	1.54	0.89
1:F:5:ILE:HB	1:F:30:ILE:HG23	1.54	0.89
1:D:7:GLY:HA3	1:D:96:THR:HG22	1.53	0.89
1:E:262:SER:O	1:E:267:LEU:HB2	1.73	0.88
2:N:70:THR:HB	2:N:73:CYS:SG	2.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:O	1:H:111:ALA:HB1	1.74	0.88
1:F:250:THR:HG23	1:F:299:VAL:HG11	1.53	0.88
1:G:130:VAL:HG21	1:G:320:ARG:HD3	1.53	0.88
1:F:117:ILE:HA	1:F:144:ILE:CD1	2.04	0.87
1:H:1:LEU:HD11	1:H:90:ASP:HB2	1.52	0.87
1:A:300:MET:HB2	1:C:226:ASN:ND2	1.90	0.87
2:K:78:ASN:HD21	1:O:231:ARG:HE	1.17	0.87
1:G:130:VAL:CG2	1:G:320:ARG:HD3	2.05	0.87
1:D:83:PRO:O	1:D:87:LEU:HB2	1.75	0.86
1:Q:210:ALA:O	1:Q:214:VAL:HG23	1.75	0.86
1:C:183:ARG:NE	1:C:187:ALA:HB3	1.89	0.86
1:G:271:LEU:HD12	1:G:272:ASP:H	1.40	0.86
1:B:204:VAL:HG22	1:D:279:VAL:HG11	1.58	0.86
1:E:60:SER:OG	1:E:65:SER:HB2	1.74	0.86
3:H:401:NAD:N7A	2:N:69:GLU:HG2	1.90	0.86
1:Q:4:ALA:HB2	1:Q:89:ILE:HG12	1.56	0.86
1:E:194:ARG:HH11	1:E:205:PRO:HB2	1.40	0.86
1:O:159:LYS:O	1:O:163:GLN:HG3	1.74	0.86
1:H:299:VAL:HG22	1:H:305:VAL:HG22	1.58	0.85
1:H:126:PRO:HB2	1:H:144:ILE:HG22	1.59	0.85
1:E:173:THR:HG22	1:E:241:ASP:HB3	1.56	0.85
1:F:183:ARG:HE	1:F:187:ALA:HB3	1.41	0.85
1:Q:133:ASN:HD22	1:Q:133:ASN:H	1.25	0.84
1:O:6:ASN:HD21	1:O:31:ASN:HD22	1.23	0.84
1:F:233:PRO:HG2	1:H:234:THR:HG22	1.60	0.84
1:H:70:ILE:C	1:H:71:ILE:HD12	1.97	0.84
1:E:300:MET:HB2	1:G:169:LYS:NZ	1.92	0.83
1:G:177:SER:HB3	1:G:234:THR:O	1.77	0.83
1:G:239:VAL:HG23	1:G:309:ALA:O	1.78	0.83
1:H:231:ARG:HG3	1:H:231:ARG:HH11	1.44	0.83
1:E:210:ALA:O	1:E:214:VAL:HG23	1.78	0.83
2:K:69:GLU:CG	1:O:77:ARG:NH2	2.41	0.83
1:E:163:GLN:O	1:E:164:LYS:HD2	1.77	0.82
2:I:62:GLU:HA	2:I:65:LYS:HE3	1.60	0.82
1:H:154:LEU:HD13	1:H:240:VAL:HG11	1.61	0.82
1:F:129:VAL:H	1:F:133:ASN:HD21	1.24	0.82
1:D:129:VAL:HG23	1:D:217:VAL:HG11	1.61	0.82
1:A:100:VAL:HG12	1:A:118:ILE:HG21	1.61	0.82
1:D:3:VAL:HG21	1:D:25:LEU:HB3	1.62	0.82
1:E:154:LEU:HD23	1:E:214:VAL:HG21	1.62	0.82
1:E:4:ALA:O	1:E:93:ILE:HD12	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:ALA:HB1	1:G:226:ASN:HA	1.60	0.82
1:C:84:TRP:HA	1:C:89:ILE:HD13	1.59	0.82
1:D:16:LEU:HD23	1:D:16:LEU:O	1.80	0.82
2:L:70:THR:HG22	2:L:71:ASN:OD1	1.78	0.82
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.62	0.81
1:G:131:GLY:H	1:G:134:ALA:HB2	1.45	0.81
1:G:157:PHE:HE1	1:G:242:LEU:HD22	1.45	0.81
1:E:194:ARG:NH2	1:G:277:PRO:HA	1.95	0.81
1:G:129:VAL:H	1:G:133:ASN:HD21	1.27	0.81
1:G:231:ARG:NH2	2:M:78:ASN:HD22	1.77	0.81
1:H:91:ILE:HD13	1:H:92:VAL:N	1.96	0.81
1:H:168:ILE:HG22	1:H:169:LYS:HG2	1.63	0.81
1:G:293:ASP:HB3	1:G:296:LEU:HD12	1.63	0.80
1:A:202:ASN:HD21	1:C:281:VAL:CG1	1.92	0.80
1:G:130:VAL:HA	1:G:134:ALA:HB2	1.64	0.80
1:D:249:LYS:HD2	1:D:302:ASP:HB3	1.61	0.80
1:C:156:PRO:HB2	1:C:290:THR:HG21	1.64	0.80
1:D:170:GLY:HA3	1:D:244:VAL:HG12	1.64	0.80
1:O:260:ARG:O	1:O:264:GLU:HG3	1.80	0.80
1:D:15:PHE:CE2	1:D:93:ILE:HG13	2.17	0.80
1:E:28:ILE:HA	1:E:71:ILE:HD12	1.64	0.80
1:F:156:PRO:HB2	1:F:290:THR:HG21	1.62	0.80
1:G:79:PRO:HA	1:G:82:LEU:HD12	1.63	0.80
1:F:117:ILE:CA	1:F:144:ILE:HD11	2.11	0.80
1:G:256:ASN:HD22	1:G:256:ASN:N	1.80	0.80
1:H:164:LYS:N	1:H:164:LYS:HD2	1.97	0.80
1:F:277:PRO:HB2	1:H:194:ARG:HG3	1.65	0.80
1:F:41:SER:HB2	1:F:64:ILE:HG21	1.62	0.80
1:F:78:ASN:HB3	1:F:81:LEU:HD13	1.63	0.79
1:F:202:ASN:HD22	1:H:281:VAL:CG2	1.96	0.79
1:F:4:ALA:HB3	1:F:92:VAL:HG22	1.65	0.79
1:G:14:ASN:OD1	1:G:50:LEU:HD11	1.82	0.79
1:H:72:GLN:H	1:H:72:GLN:HE21	1.30	0.79
1:F:67:ASP:HB2	1:F:69:LYS:HE2	1.64	0.79
2:L:57:SER:OG	2:L:58:ASP:N	2.12	0.79
1:H:293:ASP:HB3	1:H:296:LEU:HD12	1.63	0.79
1:D:318:SER:O	1:D:322:VAL:HG23	1.83	0.79
1:E:119:THR:HG22	1:E:321:VAL:HG11	1.65	0.79
1:E:169:LYS:HE3	1:G:303:ASP:OD2	1.83	0.78
1:G:28:ILE:H	1:G:28:ILE:HD13	1.49	0.78
1:B:139:HIS:HB3	1:B:333:LYS:CE	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:149:CYS:HB3	3:F:401:NAD:H5N	1.64	0.78
1:F:301:GLY:HA3	1:H:169:LYS:HD2	1.66	0.78
1:D:20:ARG:HH21	1:D:319:GLN:NE2	1.82	0.78
1:E:84:TRP:HD1	1:E:113:ALA:HB2	1.48	0.78
2:I:58:ASP:OD1	2:I:61:GLU:HG3	1.84	0.78
1:A:37:VAL:HG21	1:A:63:ALA:H	1.48	0.78
1:C:21:LYS:H	1:C:21:LYS:HD2	1.49	0.78
1:F:271:LEU:HD12	1:F:272:ASP:H	1.48	0.78
2:N:58:ASP:HA	2:N:61:GLU:OE1	1.82	0.78
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.18	0.78
1:B:185:LEU:HD21	1:C:178:TYR:HE1	1.48	0.78
1:B:208:THR:HG23	1:B:209:GLY:N	1.98	0.78
1:D:139:HIS:HB3	1:D:333:LYS:HE2	1.64	0.78
1:Q:126:PRO:HG2	1:Q:141:GLU:HG2	1.64	0.78
1:C:76:ASN:OD1	1:C:81:LEU:HD12	1.84	0.77
1:F:176:HIS:HA	1:F:238:SER:CB	2.13	0.77
1:C:89:ILE:H	1:C:89:ILE:HD12	1.49	0.77
1:E:153:CYS:HA	1:E:290:THR:HG22	1.67	0.77
1:F:56:ASP:HB2	1:F:67:ASP:H	1.50	0.77
2:K:58:ASP:O	2:K:62:GLU:HG3	1.83	0.77
1:F:56:ASP:O	1:F:66:VAL:HA	1.85	0.77
1:F:96:THR:OG1	1:F:98:VAL:HG22	1.83	0.77
1:H:91:ILE:HD13	1:H:92:VAL:H	1.49	0.77
2:M:57:SER:O	2:M:61:GLU:HB2	1.82	0.77
1:A:281:VAL:H	1:C:202:ASN:ND2	1.81	0.77
1:O:129:VAL:H	1:O:133:ASN:HD21	1.33	0.77
1:A:184:LEU:HG	1:A:185:LEU:HD12	1.67	0.77
1:F:126:PRO:HG2	1:F:144:ILE:HG22	1.66	0.77
1:H:2:LYS:HD2	1:H:88:GLY:CA	2.15	0.77
1:O:33:THR:HG22	1:O:77:ARG:HG2	1.65	0.77
1:B:191:ARG:HH21	2:J:61:GLU:HA	1.49	0.77
1:E:186:ASP:HB3	1:H:13:ARG:HH22	1.50	0.77
1:E:63:ALA:HA	1:E:73:VAL:HG23	1.67	0.77
1:F:245:GLN:HE21	1:H:245:GLN:HE21	1.31	0.76
1:F:38:LYS:HD3	2:M:57:SER:CA	2.14	0.76
1:A:65:SER:HB3	1:A:70:ILE:CD1	2.15	0.76
1:Q:28:ILE:HD11	1:Q:89:ILE:HD11	1.65	0.76
1:F:117:ILE:HG23	1:F:144:ILE:HD11	1.67	0.76
1:O:129:VAL:H	1:O:133:ASN:ND2	1.83	0.76
1:D:89:ILE:HG21	1:D:92:VAL:HG23	1.65	0.76
1:E:133:ASN:OD1	1:E:217:VAL:HA	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LYS:O	1:B:163:GLN:HB2	1.87	0.75
1:C:260:ARG:O	1:C:264:GLU:HG2	1.86	0.75
1:G:155:ALA:HB3	1:G:156:PRO:HD3	1.67	0.75
1:E:109:ILE:HA	1:E:113:ALA:HB3	1.66	0.75
1:F:289:SER:OG	1:F:320:ARG:HD2	1.86	0.75
1:G:139:HIS:CE1	1:G:332:TRP:HA	2.22	0.75
2:K:69:GLU:CG	1:O:77:ARG:HH22	1.97	0.75
1:A:96:THR:OG1	1:A:98:VAL:HG22	1.87	0.75
1:G:273:VAL:HG13	1:G:292:ILE:HG22	1.69	0.75
1:C:330:ASN:HD22	1:C:330:ASN:N	1.84	0.75
1:G:323:ASP:O	1:G:327:ILE:HD13	1.87	0.75
1:H:130:VAL:HA	1:H:134:ALA:HB2	1.68	0.75
1:E:235:PRO:HG2	1:E:284:ARG:HH21	1.51	0.75
1:D:7:GLY:CA	1:D:96:THR:HG22	2.16	0.75
1:G:79:PRO:HA	1:G:82:LEU:CD1	2.17	0.75
1:E:80:SER:HB2	1:E:107:LYS:HE2	1.68	0.75
1:E:80:SER:CB	1:E:107:LYS:HE2	2.17	0.75
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.21	0.75
1:H:176:HIS:HA	1:H:238:SER:HB3	1.67	0.75
1:Q:90:ASP:HA	1:Q:114:LYS:HD2	1.69	0.75
1:B:139:HIS:CB	1:B:333:LYS:HE2	2.15	0.74
1:A:300:MET:CE	1:C:226:ASN:HD22	2.00	0.74
1:E:263:ALA:O	1:E:268:LYS:HA	1.87	0.74
1:E:267:LEU:HD13	1:E:271:LEU:HD13	1.69	0.74
1:A:156:PRO:HB2	1:A:290:THR:HG21	1.69	0.74
1:D:251:PHE:O	1:D:255:VAL:HG23	1.87	0.74
1:F:10:ARG:O	1:F:14:ASN:HB2	1.87	0.74
1:E:279:VAL:HG22	1:G:197:ARG:NH1	2.03	0.74
1:G:168:ILE:HB	1:G:245:GLN:O	1.87	0.74
1:B:181:ASP:OD2	2:J:76:TYR:HB2	1.86	0.74
1:A:203:ILE:HB	1:C:280:SER:HB3	1.69	0.74
1:F:172:MET:O	1:F:227:GLY:HA3	1.88	0.74
1:F:21:LYS:H	1:F:21:LYS:NZ	1.86	0.74
1:G:256:ASN:ND2	1:G:256:ASN:N	2.35	0.74
1:D:215:ALA:HB1	1:D:222:LYS:HA	1.70	0.74
1:D:78:ASN:HD22	1:D:81:LEU:CG	1.95	0.74
1:D:301:GLY:O	1:D:302:ASP:HB2	1.87	0.74
1:E:186:ASP:HB3	1:H:13:ARG:NH2	2.02	0.74
1:E:275:ASP:HA	1:E:294:SER:OG	1.88	0.74
2:K:71:ASN:HA	2:K:74:ARG:HH21	1.51	0.74
1:A:129:VAL:H	1:A:133:ASN:ND2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:MET:HB2	1:C:226:ASN:HD21	1.51	0.74
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.69	0.74
1:C:129:VAL:H	1:C:133:ASN:ND2	1.86	0.74
1:E:217:VAL:HG23	1:E:218:LEU:HG	1.69	0.73
1:F:129:VAL:H	1:F:133:ASN:ND2	1.86	0.73
1:H:269:GLY:HA2	1:H:288:PHE:HE2	1.53	0.73
1:F:190:HIS:HB3	1:F:196:ALA:HB2	1.70	0.73
1:D:106:GLY:O	1:D:109:ILE:HG12	1.88	0.73
1:D:194:ARG:NH1	1:D:205:PRO:HB2	2.04	0.73
1:E:318:SER:O	1:E:322:VAL:HG23	1.88	0.73
1:E:32:ASP:C	1:E:34:GLY:H	1.91	0.73
1:G:271:LEU:HD11	1:G:292:ILE:CD1	2.17	0.73
1:O:39:GLN:NE2	1:O:39:GLN:H	1.87	0.73
1:H:117:ILE:HD11	1:H:324:LEU:HD23	1.70	0.73
1:F:251:PHE:CE1	1:F:254:GLU:HB2	2.23	0.73
1:G:161:LEU:CB	1:G:167:ILE:HD11	2.09	0.73
1:H:206:THR:HG23	1:H:229:ALA:HB3	1.70	0.73
1:E:3:VAL:HG21	1:E:25:LEU:HD22	1.70	0.73
1:O:154:LEU:HD23	1:O:240:VAL:HG11	1.70	0.73
1:D:242:LEU:HD12	1:D:243:VAL:N	2.04	0.72
1:G:133:ASN:OD1	1:G:217:VAL:HG12	1.89	0.72
1:E:115:LYS:NZ	1:E:115:LYS:HB3	2.04	0.72
1:E:186:ASP:HB2	1:H:10:ARG:HH12	1.52	0.72
1:B:296:LEU:HD22	1:D:228:ILE:HG21	1.69	0.72
1:C:272:ASP:O	1:C:291:THR:HA	1.89	0.72
1:D:152:ASN:ND2	1:D:320:ARG:HG3	2.04	0.72
1:F:90:ASP:HA	1:F:114:LYS:HD3	1.72	0.72
1:G:203:ILE:HG23	1:G:232:VAL:HG12	1.72	0.72
1:G:83:PRO:O	1:G:87:LEU:HD22	1.89	0.72
1:E:84:TRP:CD1	1:E:113:ALA:HB2	2.23	0.72
1:F:187:ALA:O	1:F:196:ALA:HB1	1.88	0.72
2:L:58:ASP:N	2:L:59:PRO:HD3	2.03	0.72
1:E:32:ASP:OD2	3:E:401:NAD:H1B	1.89	0.72
1:D:176:HIS:HA	1:D:238:SER:HB3	1.70	0.72
1:C:177:SER:HB3	1:C:234:THR:O	1.89	0.72
1:D:161:LEU:HD21	1:D:259:PHE:CZ	2.25	0.71
1:H:84:TRP:CD1	1:H:111:ALA:HB3	2.25	0.71
1:O:154:LEU:O	1:O:158:VAL:HG23	1.90	0.71
1:D:78:ASN:ND2	1:D:81:LEU:HG	1.96	0.71
1:G:129:VAL:HG23	1:G:217:VAL:HG11	1.71	0.71
1:F:114:LYS:N	1:F:114:LYS:HD2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ILE:O	1:E:28:ILE:HD13	1.91	0.71
1:G:271:LEU:HD12	1:G:272:ASP:N	2.04	0.71
1:E:298:MET:SD	1:G:226:ASN:ND2	2.64	0.71
1:Q:168:ILE:HD11	1:Q:247:SER:HB3	1.73	0.71
1:D:242:LEU:HD11	1:D:244:VAL:HG13	1.72	0.71
1:A:300:MET:HE2	1:C:226:ASN:HD22	1.53	0.70
1:E:235:PRO:HG2	1:E:284:ARG:NH2	2.05	0.70
1:F:130:VAL:HB	1:F:320:ARG:HD3	1.72	0.70
1:G:202:ASN:O	1:G:233:PRO:HD3	1.90	0.70
1:O:202:ASN:HD21	1:Q:281:VAL:HG12	1.55	0.70
1:E:25:LEU:HD21	1:E:325:ALA:O	1.91	0.70
1:A:279:VAL:HG22	1:C:197:ARG:NH1	2.06	0.70
1:H:73:VAL:O	1:H:73:VAL:HG12	1.92	0.70
2:L:71:ASN:N	2:L:71:ASN:OD1	2.23	0.70
1:E:239:VAL:HG22	1:E:240:VAL:H	1.55	0.70
1:H:37:VAL:HG21	1:H:62:THR:HA	1.72	0.70
1:H:191:ARG:HG3	2:N:73:CYS:HA	1.72	0.70
1:B:93:ILE:HD13	1:B:117:ILE:CG2	2.22	0.70
1:C:102:ARG:HG3	1:C:102:ARG:HH11	1.57	0.70
1:C:63:ALA:HB1	1:C:70:ILE:HD11	1.74	0.70
1:A:14:ASN:OD1	1:A:50:LEU:HD11	1.92	0.69
1:H:155:ALA:HB3	1:H:156:PRO:HD3	1.71	0.69
1:H:231:ARG:HG3	1:H:231:ARG:NH1	2.06	0.69
1:H:249:LYS:HG2	1:H:302:ASP:HB3	1.74	0.69
1:B:202:ASN:HD21	1:D:281:VAL:HB	1.57	0.69
1:H:1:LEU:CD1	1:H:90:ASP:HB2	2.22	0.69
1:B:114:LYS:HZ3	1:B:332:TRP:HZ2	1.39	0.69
1:B:139:HIS:HB2	1:B:333:LYS:HG3	1.73	0.69
1:D:236:ASN:OD1	1:D:314:GLU:HG3	1.92	0.69
1:G:205:PRO:HB3	1:G:230:LEU:HD23	1.73	0.69
1:A:105:ALA:HB1	1:A:116:VAL:HG11	1.74	0.69
1:E:169:LYS:HD2	1:G:301:GLY:CA	2.22	0.69
1:G:251:PHE:C	1:G:299:VAL:HG21	2.12	0.69
1:F:32:ASP:OD1	3:F:401:NAD:H1B	1.92	0.69
1:F:300:MET:CG	1:H:226:ASN:HD21	2.06	0.69
1:E:60:SER:HG	1:E:65:SER:HB2	1.54	0.69
1:D:313:ASN:O	3:D:401:NAD:H4N	1.93	0.69
1:B:31:ASN:HB2	1:B:74:VAL:CG2	2.23	0.69
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.28	0.69
1:A:298:MET:HE1	1:C:226:ASN:HB2	1.75	0.69
1:D:262:SER:HB3	1:D:267:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:PHE:HE2	1:E:27:ILE:HD11	1.58	0.68
1:E:319:GLN:OE1	1:E:319:GLN:HA	1.92	0.68
1:F:154:LEU:O	1:F:158:VAL:HG23	1.93	0.68
1:H:181:ASP:HB3	1:H:195:ARG:CD	2.22	0.68
2:N:58:ASP:HB3	2:N:59:PRO:HD3	1.75	0.68
1:A:157:PHE:HB2	1:A:259:PHE:CE1	2.28	0.68
1:E:159:LYS:O	1:E:163:GLN:HB2	1.93	0.68
1:E:80:SER:HB2	1:E:107:LYS:CE	2.23	0.68
1:H:32:ASP:OD1	3:H:401:NAD:H1B	1.92	0.68
1:O:6:ASN:HD21	1:O:31:ASN:ND2	1.91	0.68
1:O:281:VAL:HG23	1:Q:202:ASN:ND2	2.08	0.68
1:H:144:ILE:H	1:H:144:ILE:HD13	1.59	0.68
1:A:0:LYS:H3	1:A:0:LYS:HE2	1.57	0.68
1:B:253:GLU:O	1:B:257:ALA:HB2	1.93	0.68
1:H:17:ARG:HG2	1:H:53:PHE:CE1	2.29	0.68
2:K:69:GLU:HG3	1:O:77:ARG:NH2	2.09	0.68
1:E:144:ILE:H	1:E:144:ILE:HD13	1.58	0.68
1:H:79:PRO:HG2	1:H:99:PHE:CZ	2.28	0.68
1:E:280:SER:HB3	1:G:203:ILE:H	1.59	0.68
1:F:279:VAL:HG23	1:F:281:VAL:HG12	1.74	0.68
1:H:272:ASP:OD2	1:H:273:VAL:N	2.26	0.68
1:A:100:VAL:HG12	1:A:118:ILE:CG2	2.24	0.68
1:B:190:HIS:HB3	1:B:196:ALA:HB2	1.75	0.68
1:D:194:ARG:HH11	1:D:205:PRO:HB2	1.59	0.68
1:B:202:ASN:HD21	1:D:281:VAL:CG1	2.07	0.68
1:F:108:HIS:HB2	1:F:116:VAL:HG21	1.75	0.68
1:G:157:PHE:CE1	1:G:242:LEU:HD22	2.29	0.68
1:B:186:ASP:HB2	1:C:10:ARG:HH11	1.57	0.68
1:F:210:ALA:HA	1:F:213:ALA:HB3	1.75	0.68
1:B:126:PRO:HG2	1:B:144:ILE:HG22	1.75	0.67
1:C:169:LYS:HE2	1:C:245:GLN:OE1	1.94	0.67
1:B:220:ASN:O	1:B:222:LYS:N	2.25	0.67
1:E:106:GLY:O	1:E:110:GLU:HG2	1.94	0.67
1:H:65:SER:HA	1:H:70:ILE:HA	1.76	0.67
1:O:202:ASN:HD21	1:Q:281:VAL:CG1	2.07	0.67
1:D:156:PRO:HB2	1:D:290:THR:HG21	1.76	0.67
1:G:324:LEU:O	1:G:328:VAL:HG23	1.93	0.67
1:F:183:ARG:NE	1:F:187:ALA:HB3	2.10	0.67
1:H:36:GLY:H	1:H:39:GLN:NE2	1.92	0.67
1:D:155:ALA:HB3	1:D:156:PRO:HD3	1.76	0.67
1:E:55:ALA:O	1:E:57:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:VAL:HA	1:G:118:ILE:HD13	1.77	0.67
1:O:122(A):LYS:HD2	5:O:535:HOH:O	1.93	0.67
1:O:226:ASN:HB2	1:Q:300:MET:HE3	1.76	0.67
1:D:124:ASP:O	1:D:125:ILE:HB	1.92	0.67
1:E:117:ILE:HD11	1:E:328:VAL:HG21	1.76	0.67
1:E:63:ALA:CB	1:E:72:GLN:HA	2.24	0.67
1:F:39:GLN:HE22	2:M:60:LEU:HD23	1.59	0.67
1:B:271:LEU:HD13	1:B:272:ASP:N	2.09	0.67
1:F:159:LYS:HB2	1:F:218:LEU:HD11	1.76	0.67
1:F:280:SER:OG	1:H:202:ASN:HB2	1.94	0.67
1:H:2:LYS:HD3	1:H:28:ILE:HD12	1.76	0.67
1:H:215:ALA:CB	1:H:222:LYS:HA	2.24	0.67
1:H:45:LYS:HB2	1:H:57:VAL:HB	1.76	0.67
1:F:194:ARG:HD2	1:F:205:PRO:O	1.94	0.67
1:O:281:VAL:H	1:Q:202:ASN:HD22	1.42	0.67
1:D:272:ASP:HB2	1:D:288:PHE:CD2	2.29	0.66
1:F:0:LYS:HD2	1:F:24:PRO:HA	1.77	0.66
1:F:234:THR:HG22	1:H:233:PRO:HG2	1.75	0.66
2:K:71:ASN:HA	2:K:74:ARG:NH2	2.09	0.66
1:O:126:PRO:HG2	1:O:141:GLU:HG2	1.76	0.66
1:E:139:HIS:CE1	1:E:332:TRP:HA	2.30	0.66
2:L:63:TYR:OH	2:L:70:THR:HB	1.94	0.66
1:E:31:ASN:OD1	1:E:74:VAL:HG23	1.96	0.66
1:F:245:GLN:NE2	1:H:245:GLN:HE21	1.92	0.66
1:Q:331:ASN:ND2	1:Q:331:ASN:N	2.41	0.66
1:A:125:ILE:HG21	1:A:143:ILE:HG22	1.78	0.66
1:A:210:ALA:O	1:A:214:VAL:HG23	1.95	0.66
1:E:239:VAL:HG22	1:E:240:VAL:N	2.10	0.66
1:F:37:VAL:HG22	1:F:73:VAL:HB	1.76	0.66
1:H:60(A):GLY:O	1:H:61:GLU:HG2	1.96	0.66
1:Q:272:ASP:O	1:Q:291:THR:HA	1.96	0.66
1:A:168:ILE:HG22	1:A:169:LYS:HG2	1.77	0.66
1:A:271:LEU:HD12	1:A:272:ASP:N	2.10	0.66
1:E:154:LEU:O	1:E:158:VAL:HG23	1.94	0.66
1:E:296:LEU:HD23	1:E:296:LEU:N	2.11	0.66
1:Q:2:LYS:HD2	1:Q:88:GLY:O	1.96	0.66
1:D:215:ALA:O	1:D:216:LEU:HD23	1.96	0.66
1:F:108:HIS:O	1:F:111:ALA:HB3	1.96	0.66
1:H:102:ARG:HH21	1:H:124:ASP:HB3	1.60	0.66
1:A:139:HIS:HB3	1:A:333:LYS:HE2	1.78	0.66
1:B:133:ASN:OD1	1:B:217:VAL:HA	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASN:HD21	1:D:281:VAL:CB	2.08	0.66
1:F:37:VAL:HG13	1:F:64:ILE:HG23	1.78	0.66
1:F:117:ILE:HG23	1:F:144:ILE:CD1	2.26	0.66
1:F:133:ASN:OD1	1:F:217:VAL:HG12	1.95	0.66
1:G:158:VAL:HG11	1:G:221:LEU:CD2	2.25	0.66
1:H:76:ASN:HD22	1:H:77:ARG:N	1.94	0.66
1:A:78:ASN:ND2	1:A:81:LEU:HG	2.10	0.66
1:E:115:LYS:HE3	1:E:137:TYR:OH	1.96	0.66
1:H:181:ASP:CG	2:N:76:TYR:H	1.99	0.66
1:B:279:VAL:CG1	1:D:204:VAL:HG13	2.26	0.65
1:D:59:PRO:HA	1:D:64:ILE:HA	1.78	0.65
1:E:183:ARG:NE	1:E:187:ALA:HB3	2.11	0.65
1:G:129:VAL:H	1:G:133:ASN:ND2	1.93	0.65
1:O:190:HIS:HB3	1:O:196:ALA:HB2	1.78	0.65
1:B:284:ARG:HD2	5:B:520:HOH:O	1.97	0.65
1:C:168:ILE:HG22	1:C:169:LYS:HD2	1.76	0.65
1:F:129:VAL:N	1:F:133:ASN:HD21	1.94	0.65
1:G:161:LEU:HD13	1:G:244:VAL:HG21	1.78	0.65
1:H:205:PRO:HA	1:H:230:LEU:HD23	1.78	0.65
3:H:401:NAD:C8A	2:N:69:GLU:HG2	2.26	0.65
1:B:277:PRO:HA	1:D:194:ARG:HH21	1.62	0.65
1:B:202:ASN:ND2	1:D:281:VAL:H	1.95	0.65
1:D:303:ASP:O	1:D:305:VAL:HG23	1.96	0.65
1:G:-1:ALA:HB2	5:G:513:HOH:O	1.97	0.65
1:E:202:ASN:CB	1:G:281:VAL:HG23	2.24	0.65
1:H:83:PRO:HB2	1:H:86:GLU:HG2	1.79	0.65
1:Q:129:VAL:H	1:Q:133:ASN:HD21	1.44	0.65
1:D:323:ASP:C	1:D:325:ALA:H	1.99	0.65
1:D:64:ILE:HG23	1:D:73:VAL:HG21	1.78	0.65
1:H:85:LYS:CA	1:H:112:GLY:HA3	2.26	0.65
1:A:115:LYS:HD2	1:A:332:TRP:CZ3	2.31	0.65
1:D:89:ILE:HG21	1:D:92:VAL:CG2	2.27	0.65
1:F:242:LEU:HD21	1:F:244:VAL:HG13	1.78	0.65
1:E:296:LEU:HD21	1:G:194:ARG:NH2	2.11	0.65
1:A:129:VAL:H	1:A:133:ASN:HD21	1.42	0.65
1:C:190:HIS:HB3	1:C:196:ALA:HB2	1.78	0.65
1:E:328:VAL:O	1:E:332:TRP:HB2	1.96	0.65
1:B:208:THR:CG2	1:B:209:GLY:H	2.00	0.65
1:D:144:ILE:HD12	1:D:145:SER:N	2.11	0.65
1:E:133:ASN:N	1:E:133:ASN:HD22	1.95	0.65
1:H:170:GLY:HA3	1:H:244:VAL:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ASN:ND2	1:H:281:VAL:HG23	2.11	0.65
1:O:102:ARG:NH2	1:O:124:ASP:O	2.30	0.65
1:B:281:VAL:HG12	1:D:202:ASN:HD21	1.61	0.64
1:D:89:ILE:CG2	1:D:92:VAL:HG23	2.26	0.64
1:G:179:THR:C	1:G:181:ASP:H	1.99	0.64
1:B:10:ARG:HH11	1:C:186:ASP:HB2	1.63	0.64
1:E:3:VAL:HG22	1:E:91:ILE:HG23	1.77	0.64
1:F:0:LYS:NZ	1:F:24:PRO:HG3	2.13	0.64
1:G:204:VAL:O	1:G:231:ARG:N	2.29	0.64
1:E:240:VAL:CG2	1:E:309:ALA:HB3	2.28	0.64
1:E:17:ARG:NH2	1:E:53:PHE:HB2	2.12	0.64
1:C:276:GLU:HB2	1:C:278:LEU:HG	1.80	0.64
1:G:28:ILE:HD11	1:G:89:ILE:CD1	2.26	0.64
1:H:190:HIS:HB3	1:H:196:ALA:HB2	1.77	0.64
1:A:154:LEU:HD22	1:A:172:MET:HE3	1.78	0.64
1:A:63:ALA:HA	1:A:73:VAL:HG23	1.80	0.64
1:B:130:VAL:HB	1:B:320:ARG:HD3	1.80	0.64
1:G:129:VAL:CG2	1:G:217:VAL:HG11	2.26	0.64
1:G:62:THR:HG22	1:Q:62:THR:HG22	1.80	0.64
1:H:164:LYS:H	1:H:164:LYS:HD2	1.60	0.64
1:G:273:VAL:HG22	1:G:292:ILE:HB	1.79	0.64
1:H:72:GLN:H	1:H:72:GLN:NE2	1.95	0.64
1:O:181:ASP:OD2	1:O:195:ARG:NH1	2.30	0.64
1:A:1:LEU:HD23	1:A:91:ILE:HD11	1.80	0.64
1:A:84:TRP:CE3	1:A:89:ILE:HG13	2.33	0.64
1:E:300:MET:HB2	1:G:169:LYS:HZ3	1.62	0.64
1:G:251:PHE:O	1:G:255:VAL:HG23	1.97	0.64
1:E:42:HIS:CG	1:H:193:LEU:HD13	2.32	0.64
1:H:263:ALA:O	1:H:268:LYS:HA	1.97	0.64
1:A:76:ASN:HD22	1:A:77:ARG:N	1.96	0.64
1:B:0:LYS:N	5:B:526:HOH:O	2.31	0.64
1:B:221:LEU:HA	1:B:224:LYS:HD2	1.80	0.64
1:E:132:VAL:HG21	1:E:155:ALA:HB1	1.79	0.64
1:A:9:GLY:HA3	3:A:401:NAD:O5B	1.98	0.64
1:B:90:ASP:HA	1:B:114:LYS:HZ2	1.62	0.64
1:C:271:LEU:HD12	1:C:272:ASP:H	1.63	0.64
1:B:18(A):TRP:CE2	1:B:27:ILE:HD13	2.32	0.63
1:D:251:PHE:CZ	1:D:254:GLU:HB2	2.33	0.63
1:D:87:LEU:HD12	1:D:89:ILE:HD13	1.79	0.63
1:F:52:ILE:HD12	1:F:52:ILE:H	1.62	0.63
1:C:34:GLY:HA2	2:J:60:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:LEU:HD11	1:E:244:VAL:CG1	2.27	0.63
1:F:113:ALA:C	1:F:114:LYS:HD2	2.19	0.63
1:E:194:ARG:HE	1:G:277:PRO:CA	2.10	0.63
1:F:301:GLY:HA3	1:H:169:LYS:CD	2.28	0.63
1:B:165:PHE:O	1:B:246:VAL:HB	1.98	0.63
1:D:18(A):TRP:CH2	1:D:69:LYS:HE2	2.32	0.63
1:B:202:ASN:HD22	1:D:281:VAL:H	1.45	0.63
1:D:275:ASP:HA	1:D:294:SER:OG	1.98	0.63
1:E:242:LEU:HD11	1:E:244:VAL:HG13	1.78	0.63
1:D:18(A):TRP:HH2	1:D:69:LYS:HE2	1.63	0.63
1:E:109:ILE:HA	1:E:113:ALA:O	1.98	0.63
1:F:21:LYS:HZ1	1:F:21:LYS:H	1.44	0.63
1:F:87:LEU:HB2	1:F:89:ILE:HG12	1.79	0.63
1:G:133:ASN:N	1:G:133:ASN:HD22	1.96	0.63
1:O:98:VAL:HG23	1:O:99:PHE:CE2	2.33	0.63
1:C:262:SER:HA	1:C:266:GLU:OE1	1.99	0.63
1:E:9:GLY:O	1:E:13:ARG:HG3	1.98	0.63
1:F:307:VAL:C	1:F:308:ILE:HD12	2.19	0.63
1:O:2:LYS:HD3	1:O:28:ILE:HD13	1.79	0.63
1:B:91:ILE:HG13	1:B:92:VAL:N	2.13	0.63
1:D:100:VAL:HG23	1:D:122(A):LYS:HB2	1.81	0.63
1:D:54:ASP:O	1:D:55:ALA:HB2	1.98	0.63
1:E:70:ILE:H	1:E:70:ILE:CD1	2.10	0.63
1:F:38:LYS:CD	2:M:57:SER:HA	2.23	0.63
1:O:39:GLN:HE21	1:O:39:GLN:H	1.45	0.63
1:B:70:ILE:HD12	1:B:70:ILE:N	2.14	0.63
1:B:10:ARG:NH1	1:C:186:ASP:HB2	2.14	0.63
1:A:271:LEU:HD12	1:A:272:ASP:H	1.64	0.63
1:B:105:ALA:HB1	1:B:116:VAL:HG11	1.81	0.63
1:D:95:GLY:HA2	1:D:119:THR:OG1	1.99	0.63
1:E:20:ARG:NH2	1:E:322:VAL:HB	2.13	0.63
1:F:233:PRO:HB2	1:H:233:PRO:HB2	1.80	0.63
1:H:176:HIS:HA	1:H:238:SER:CB	2.28	0.63
2:L:63:TYR:HE2	2:L:72:GLU:HG3	1.63	0.63
1:A:28:ILE:HG22	1:A:69:LYS:CE	2.29	0.63
1:C:129:VAL:H	1:C:133:ASN:HD21	1.44	0.63
1:D:28:ILE:HD11	1:D:89:ILE:HD11	1.81	0.63
1:E:117:ILE:HG22	1:E:117:ILE:O	1.99	0.63
1:B:0:LYS:HE3	1:B:23:SER:O	1.99	0.62
1:H:3:VAL:HG21	1:H:93:ILE:HD11	1.81	0.62
1:A:159:LYS:HB2	1:A:218:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LYS:N	1:C:21:LYS:HD2	2.11	0.62
1:C:83:PRO:HB2	1:C:86:GLU:HB3	1.81	0.62
1:E:202:ASN:HB2	1:G:280:SER:OG	1.99	0.62
1:E:299:VAL:HG22	1:E:305:VAL:HA	1.80	0.62
1:B:168:ILE:HB	1:B:245:GLN:O	1.99	0.62
1:A:191:ARG:HG2	1:A:191:ARG:HH11	1.65	0.62
1:C:115:LYS:HE3	1:C:141:GLU:O	1.99	0.62
1:D:130:VAL:HA	1:D:134:ALA:HB2	1.81	0.62
1:Q:152:ASN:O	1:Q:289:SER:HB3	1.99	0.62
1:B:324:LEU:O	1:B:328:VAL:HG23	1.99	0.62
1:B:281:VAL:H	1:D:202:ASN:HD21	1.46	0.62
1:E:186:ASP:HB2	1:H:10:ARG:HH11	1.64	0.62
1:F:14:ASN:ND2	1:F:314:GLU:HG2	2.15	0.62
1:B:176:HIS:NE2	2:J:78:ASN:HB3	2.14	0.62
1:H:66:VAL:C	1:H:68:GLY:H	2.02	0.62
2:L:71:ASN:HB2	1:Q:183:ARG:NH1	2.14	0.62
1:Q:33:THR:HG21	1:Q:77:ARG:NH1	2.15	0.62
1:G:217:VAL:HG23	1:G:218:LEU:HG	1.80	0.62
1:A:171:THR:O	1:A:242:LEU:HD12	1.99	0.62
1:D:152:ASN:HD21	1:D:320:ARG:HG3	1.65	0.62
1:D:177:SER:HB3	1:D:234:THR:O	2.00	0.62
1:E:32:ASP:C	1:E:34:GLY:N	2.52	0.62
1:F:129:VAL:O	1:F:131:GLY:N	2.33	0.62
1:H:265:LYS:HE2	1:H:265:LYS:HA	1.82	0.62
1:H:79:PRO:CG	1:H:99:PHE:CZ	2.83	0.62
1:A:234:THR:HG21	1:C:203:ILE:HG12	1.80	0.62
1:D:123:GLY:HA2	5:D:528:HOH:O	1.99	0.62
1:B:90:ASP:HA	1:B:114:LYS:NZ	2.15	0.61
1:C:210:ALA:O	1:C:214:VAL:HG23	1.99	0.61
1:B:169:LYS:HD3	1:D:301:GLY:HA3	1.82	0.61
1:E:202:ASN:HB3	1:G:281:VAL:CG2	2.26	0.61
1:E:322:VAL:HG12	1:E:322:VAL:O	1.99	0.61
1:F:324:LEU:O	1:F:328:VAL:HG23	1.99	0.61
1:F:60:SER:N	1:F:64:ILE:HA	2.15	0.61
1:G:205:PRO:HA	1:G:229:ALA:O	1.99	0.61
1:F:310:TRP:HZ2	1:H:205:PRO:HG2	1.64	0.61
1:E:183:ARG:HH22	2:N:74:ARG:HH12	1.48	0.61
1:A:37:VAL:CG2	1:A:63:ALA:H	2.13	0.61
1:F:56:ASP:HB2	1:F:67:ASP:N	2.15	0.61
1:E:170:GLY:O	1:G:300:MET:HG2	2.00	0.61
1:H:24:PRO:C	1:H:25:LEU:HD12	2.20	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:CYS:O	1:A:156:PRO:HD2	2.00	0.61
1:D:159:LYS:O	1:D:163:GLN:HG2	2.00	0.61
1:E:214:VAL:O	1:E:217:VAL:HG22	1.99	0.61
1:E:153:CYS:O	1:E:290:THR:HG21	2.01	0.61
1:G:221:LEU:HD12	1:G:224:LYS:HB2	1.81	0.61
1:H:195:ARG:HB2	1:H:195:ARG:HH11	1.64	0.61
1:D:242:LEU:HD12	1:D:243:VAL:H	1.66	0.61
1:E:115:LYS:HB3	1:E:115:LYS:HZ2	1.64	0.61
1:O:21:LYS:HG2	5:O:580:HOH:O	1.99	0.61
1:B:193:LEU:HD13	1:C:42:HIS:CG	2.36	0.61
1:F:101:ASP:OD2	1:F:103:GLU:HB3	1.99	0.61
2:L:63:TYR:O	2:L:67:ASN:HB2	2.01	0.61
1:F:18(A):TRP:HA	1:F:20:ARG:HG2	1.82	0.61
1:H:246:VAL:HG22	1:H:303:ASP:O	2.01	0.61
1:H:255:VAL:O	1:H:258:ALA:HB3	2.00	0.61
1:B:18(A):TRP:CD2	1:B:27:ILE:HD13	2.35	0.61
1:F:211:ALA:HB3	5:F:501:HOH:O	2.00	0.61
1:Q:191:ARG:HG3	1:Q:191:ARG:HH11	1.65	0.61
1:B:130:VAL:HA	1:B:134:ALA:HB2	1.83	0.61
1:B:281:VAL:H	1:D:202:ASN:ND2	1.99	0.61
1:E:169:LYS:CE	1:G:303:ASP:OD2	2.48	0.61
1:F:227:GLY:HA2	1:H:298:MET:CE	2.31	0.61
1:A:280:SER:HB3	1:C:203:ILE:HD12	1.82	0.61
1:B:279:VAL:HG12	1:D:204:VAL:HA	1.82	0.61
1:B:31:ASN:HB2	1:B:74:VAL:HG23	1.83	0.61
1:D:264:GLU:O	1:D:265:LYS:HD2	2.01	0.61
1:F:133:ASN:N	1:F:133:ASN:HD22	1.99	0.61
1:F:280:SER:HB3	1:H:203:ILE:HB	1.83	0.61
2:M:76:TYR:N	2:M:76:TYR:CD1	2.69	0.61
1:Q:86:GLU:N	1:Q:86:GLU:OE2	2.30	0.61
1:A:281:VAL:H	1:C:202:ASN:HD21	1.48	0.60
1:B:204:VAL:HG22	1:D:279:VAL:CG1	2.30	0.60
1:H:126:PRO:HD2	1:H:143:ILE:O	2.00	0.60
1:C:133:ASN:C	1:C:135:ASP:H	2.05	0.60
1:A:279:VAL:HG11	1:C:204:VAL:HG22	1.82	0.60
1:G:190:HIS:HB3	1:G:196:ALA:HB2	1.81	0.60
1:H:115:LYS:HG2	1:H:142:PRO:HA	1.82	0.60
1:H:1:LEU:HD12	1:H:2:LYS:H	1.66	0.60
1:A:76:ASN:ND2	1:A:78:ASN:H	2.00	0.60
1:E:20:ARG:NH1	1:E:322:VAL:HG12	2.16	0.60
1:F:27:ILE:N	1:F:27:ILE:HD12	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:LEU:HD13	1:G:271:LEU:HB3	1.82	0.60
1:O:195:ARG:HH12	1:O:231:ARG:NH2	1.99	0.60
1:O:6:ASN:ND2	1:O:31:ASN:ND2	2.44	0.60
1:Q:6:ASN:ND2	1:Q:94:GLU:OE2	2.31	0.60
1:B:284:ARG:CZ	1:B:284:ARG:HB3	2.30	0.60
1:B:83:PRO:HG2	1:B:87:LEU:HD12	1.83	0.60
1:E:58:LYS:NZ	1:E:58:LYS:HB3	2.16	0.60
1:F:117:ILE:CG2	1:F:144:ILE:HD11	2.31	0.60
1:F:271:LEU:HD12	1:F:272:ASP:N	2.14	0.60
1:G:250:THR:O	1:G:299:VAL:HG11	2.02	0.60
1:C:133:ASN:O	1:C:135:ASP:N	2.35	0.60
1:A:298:MET:CE	1:C:226:ASN:HB2	2.30	0.60
1:D:167:ILE:HG23	1:D:244:VAL:HB	1.84	0.60
1:E:116:VAL:HB	1:E:143:ILE:HD13	1.83	0.60
1:E:239:VAL:HA	1:E:309:ALA:O	2.01	0.60
1:A:101:ASP:HB3	1:A:122(A):LYS:HB3	1.84	0.60
1:A:28:ILE:HG22	1:A:69:LYS:HE2	1.84	0.60
1:E:83:PRO:HA	1:E:86:GLU:OE1	2.01	0.60
1:H:1:LEU:HD12	1:H:2:LYS:N	2.17	0.60
1:O:243:VAL:HG11	1:Q:243:VAL:HG11	1.82	0.60
1:E:32:ASP:O	1:E:34:GLY:N	2.34	0.60
1:G:129:VAL:O	1:G:129:VAL:HG12	2.02	0.60
1:E:251:PHE:CE1	1:E:254:GLU:HB2	2.36	0.60
1:E:37:VAL:HG23	1:E:38:LYS:HE2	1.84	0.60
1:F:23:SER:C	1:F:25:LEU:H	2.05	0.60
1:F:299:VAL:HG12	1:F:299:VAL:O	2.02	0.60
1:G:170:GLY:HA3	1:G:244:VAL:HA	1.84	0.60
1:G:287:ASP:HB3	5:G:501:HOH:O	2.01	0.60
2:M:58:ASP:HB3	2:M:59:PRO:HD3	1.84	0.60
1:B:117:ILE:O	1:B:117:ILE:HG23	2.02	0.59
1:B:140:ASP:O	1:B:142:PRO:HD3	2.02	0.59
1:B:271:LEU:HD13	1:B:272:ASP:H	1.67	0.59
1:E:117:ILE:CG1	1:E:144:ILE:HD11	2.28	0.59
2:K:72:GLU:CD	2:K:72:GLU:H	2.05	0.59
1:Q:96:THR:OG1	1:Q:98:VAL:HG22	2.02	0.59
1:A:204:VAL:HB	1:A:231:ARG:HB2	1.84	0.59
1:B:250:THR:OG1	1:B:251:PHE:N	2.34	0.59
1:E:25:LEU:HD11	1:E:325:ALA:HB3	1.84	0.59
1:F:137:TYR:CE2	1:F:328:VAL:HA	2.37	0.59
1:F:169:LYS:HE3	1:H:304:MET:HB2	1.83	0.59
1:H:36:GLY:H	1:H:39:GLN:HE21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:ILE:CD1	1:O:116:VAL:HG23	2.32	0.59
1:O:172:MET:CE	1:O:211:ALA:HB2	2.32	0.59
1:Q:133:ASN:ND2	1:Q:133:ASN:H	1.98	0.59
1:C:102:ARG:HG3	1:C:102:ARG:NH1	2.17	0.59
1:E:192:ASP:HB3	1:E:195:ARG:HB2	1.84	0.59
1:G:16:LEU:O	1:G:16:LEU:HD23	2.01	0.59
1:E:16:LEU:HD13	1:E:44:LEU:HD21	1.85	0.59
1:Q:133:ASN:HD22	1:Q:133:ASN:N	1.92	0.59
1:B:317:TYR:O	1:B:321:VAL:HG23	2.02	0.59
1:D:83:PRO:O	1:D:87:LEU:CB	2.49	0.59
1:H:85:LYS:N	1:H:112:GLY:HA3	2.18	0.59
1:D:146:ASN:ND2	1:D:321:VAL:HG23	2.17	0.59
1:D:209:GLY:O	1:D:211:ALA:N	2.35	0.59
1:E:276:GLU:HG2	5:E:534:HOH:O	2.03	0.59
1:H:85:LYS:O	1:H:85:LYS:HD3	2.02	0.59
1:C:241:ASP:OD1	1:C:306:LYS:HE3	2.03	0.59
1:D:133:ASN:HD21	1:D:217:VAL:HG12	1.67	0.59
1:D:167:ILE:HA	1:D:246:VAL:HG12	1.84	0.59
1:F:227:GLY:HA2	1:H:298:MET:HE1	1.83	0.59
1:A:229:ALA:O	1:A:230:LEU:HD23	2.03	0.59
1:B:272:ASP:O	1:B:291:THR:HA	2.03	0.59
1:B:93:ILE:HD13	1:B:117:ILE:HG21	1.84	0.59
1:C:21:LYS:H	1:C:21:LYS:CD	2.14	0.59
1:C:89:ILE:HD12	1:C:89:ILE:N	2.16	0.59
1:E:157:PHE:HB2	1:E:259:PHE:CE1	2.38	0.59
1:F:171:THR:HG23	1:F:171:THR:O	2.02	0.59
1:A:101:ASP:HA	1:A:125:ILE:HD11	1.85	0.59
1:E:301:GLY:O	1:E:303:ASP:N	2.35	0.59
1:E:279:VAL:HG12	1:G:205:PRO:HD2	1.85	0.59
1:G:272:ASP:O	1:G:291:THR:HA	2.03	0.59
1:B:194:ARG:NH1	1:D:278:LEU:O	2.36	0.59
1:D:150:THR:OG1	2:I:78:ASN:HB2	2.01	0.59
1:D:211:ALA:HB1	1:D:226:ASN:CA	2.33	0.59
1:E:130:VAL:HB	1:E:320:ARG:HD3	1.85	0.59
1:E:279:VAL:HG22	1:G:197:ARG:HH12	1.66	0.59
1:F:178:TYR:HE1	1:G:185:LEU:HD21	1.68	0.59
1:Q:319:GLN:HA	1:Q:319:GLN:OE1	2.02	0.59
1:A:139:HIS:HB3	1:A:333:LYS:CE	2.33	0.58
1:D:115:LYS:HG3	1:D:142:PRO:HA	1.85	0.58
1:D:162:ASP:HA	1:D:167:ILE:HG13	1.85	0.58
1:E:119:THR:CG2	1:E:321:VAL:HG11	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:THR:HG23	1:F:145:SER:OG	2.03	0.58
1:F:270:ILE:N	1:F:270:ILE:HD12	2.18	0.58
1:H:79:PRO:HB2	1:H:107:LYS:HB3	1.84	0.58
1:H:84:TRP:HA	1:H:89:ILE:HG13	1.84	0.58
1:A:100:VAL:HA	1:A:118:ILE:HD13	1.85	0.58
1:D:133:ASN:C	1:D:135:ASP:H	2.06	0.58
1:H:203:ILE:O	1:H:205:PRO:HD3	2.03	0.58
1:Q:236:ASN:O	1:Q:237:VAL:HB	2.04	0.58
1:A:1:LEU:HD22	1:A:329:ALA:CB	2.34	0.58
1:C:18(A):TRP:O	1:C:20:ARG:HB2	2.04	0.58
1:B:279:VAL:CG2	1:D:197:ARG:HG3	2.32	0.58
1:D:94:GLU:HG3	1:D:94:GLU:O	2.03	0.58
1:E:160:VAL:CG2	1:E:267:LEU:HD11	2.34	0.58
1:E:79:PRO:HB3	1:E:108:HIS:CE1	2.39	0.58
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.39	0.58
1:F:130:VAL:HG21	1:F:320:ARG:O	2.04	0.58
1:G:162:ASP:CA	1:G:167:ILE:HG12	2.33	0.58
1:H:71:ILE:N	1:H:71:ILE:HD12	2.19	0.58
1:Q:14:ASN:OD1	1:Q:50:LEU:HD11	2.03	0.58
1:E:172:MET:HG2	1:E:173:THR:N	2.19	0.58
1:F:132:VAL:HG12	1:F:133:ASN:N	2.18	0.58
1:E:300:MET:HB3	1:G:169:LYS:HD3	1.85	0.58
1:B:87:LEU:HB2	1:B:89:ILE:HD13	1.85	0.58
1:C:98:VAL:HG23	1:C:99:PHE:CD2	2.38	0.58
1:E:300:MET:HB2	1:G:169:LYS:HZ2	1.67	0.58
1:C:228:ILE:HD13	1:C:228:ILE:H	1.68	0.58
1:D:211:ALA:HB1	1:D:226:ASN:HA	1.85	0.58
1:E:185:LEU:O	1:E:187:ALA:N	2.36	0.58
1:F:211:ALA:CB	1:F:226:ASN:HA	2.34	0.58
1:H:42:HIS:O	1:H:46:TYR:HB2	2.03	0.58
1:C:91:ILE:HD13	1:C:91:ILE:C	2.23	0.58
1:D:9:GLY:HA3	3:D:401:NAD:O5B	2.03	0.58
1:E:129:VAL:H	1:E:133:ASN:ND2	2.02	0.58
1:E:146:ASN:ND2	1:E:324:LEU:HD22	2.19	0.58
1:F:165:PHE:HD1	1:F:248:LYS:HB3	1.69	0.58
1:H:163:GLN:OE1	1:H:164:LYS:HE3	2.03	0.58
1:H:4:ALA:HB2	1:H:89:ILE:CD1	2.34	0.58
1:G:231:ARG:HH21	2:M:78:ASN:HD22	1.49	0.58
1:H:191:ARG:CG	2:N:73:CYS:HA	2.34	0.58
1:B:9:GLY:O	1:B:13:ARG:HG3	2.03	0.58
1:D:139:HIS:CD2	1:D:333:LYS:HD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:VAL:HG13	1:D:159:LYS:HD2	1.85	0.57
1:E:241:ASP:OD1	1:E:306:LYS:HE2	2.04	0.57
1:H:17:ARG:NE	1:H:53:PHE:HD1	2.01	0.57
2:N:60:LEU:O	2:N:60:LEU:HD23	2.04	0.57
1:F:101:ASP:O	1:F:104:GLY:N	2.36	0.57
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.86	0.57
1:B:197:ARG:NH2	1:C:46:TYR:HB3	2.18	0.57
1:D:20:ARG:HH21	1:D:319:GLN:HE22	1.53	0.57
1:E:60:SER:HB2	1:E:63:ALA:O	2.04	0.57
1:E:169:LYS:CD	1:G:301:GLY:HA3	2.27	0.57
2:I:70:THR:O	2:I:74:ARG:HG3	2.04	0.57
2:K:69:GLU:HG2	1:O:77:ARG:HH22	1.69	0.57
1:A:38:LYS:HD3	1:A:39:GLN:HE22	1.69	0.57
1:E:132:VAL:HG11	1:E:217:VAL:HB	1.85	0.57
1:E:295:SER:HB2	1:E:296:LEU:HD23	1.87	0.57
1:O:253:GLU:H	1:O:253:GLU:CD	2.06	0.57
2:K:69:GLU:CD	1:O:77:ARG:HH22	2.06	0.57
1:Q:181:ASP:OD2	1:Q:195:ARG:NH1	2.37	0.57
1:C:333:LYS:NZ	1:C:333:LYS:HB2	2.20	0.57
1:D:10:ARG:HB2	3:D:401:NAD:O1N	2.04	0.57
1:B:277:PRO:HB2	1:D:194:ARG:HE	1.70	0.57
1:D:133:ASN:ND2	1:D:217:VAL:HA	2.19	0.57
1:D:319:GLN:NE2	1:D:319:GLN:HA	2.20	0.57
1:E:265:LYS:HB2	1:E:266:GLU:OE1	2.05	0.57
1:G:-1:ALA:HB3	1:G:26:ASP:HB2	1.86	0.57
1:G:281:VAL:HG11	1:H:48:SER:HA	1.85	0.57
1:G:294:SER:C	1:G:296:LEU:H	2.08	0.57
1:O:202:ASN:ND2	1:Q:281:VAL:HG12	2.20	0.57
1:A:122(A):LYS:HD3	1:A:123:GLY:N	2.19	0.57
1:B:204:VAL:HA	1:D:279:VAL:HG12	1.86	0.57
1:D:55:ALA:O	1:D:57:VAL:HG23	2.03	0.57
1:G:153:CYS:O	1:G:156:PRO:HD2	2.05	0.57
1:C:77:ARG:O	1:C:79:PRO:HD3	2.05	0.57
1:E:106:GLY:O	1:E:109:ILE:HG12	2.04	0.57
1:F:221:LEU:HA	1:F:224:LYS:HD2	1.86	0.57
2:M:76:TYR:N	2:M:76:TYR:HD1	2.02	0.57
1:B:185:LEU:HD21	1:C:178:TYR:CE1	2.36	0.57
1:B:280:SER:HA	1:B:310:TRP:CZ3	2.40	0.57
1:F:29:ALA:HA	1:F:72:GLN:O	2.04	0.57
1:H:178:TYR:CE2	1:H:200:ALA:HB2	2.40	0.57
1:D:62:THR:HG21	1:H:74:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:60:LEU:HD21	2:N:64:CYS:SG	2.44	0.57
1:B:280:SER:HB3	1:D:203:ILE:HB	1.87	0.57
1:O:126:PRO:HB2	1:O:144:ILE:HG22	1.86	0.57
1:F:172:MET:HE1	1:F:211:ALA:HB2	1.85	0.57
1:F:282:ASP:OD2	1:H:197:ARG:NH1	2.34	0.57
1:G:37:VAL:HG13	1:G:73:VAL:HB	1.87	0.57
1:Q:281:VAL:O	1:Q:284:ARG:HG3	2.04	0.57
1:D:139:HIS:CD2	1:D:333:LYS:HB2	2.40	0.56
1:D:144:ILE:HD12	1:D:144:ILE:C	2.25	0.56
1:B:171:THR:HG21	1:D:306:LYS:HE3	1.87	0.56
1:D:15:PHE:CD1	1:D:322:VAL:HG22	2.40	0.56
1:D:1:LEU:HD22	1:D:329:ALA:HA	1.87	0.56
1:E:70:ILE:HD13	1:E:70:ILE:N	2.15	0.56
1:D:117:ILE:CG2	1:D:144:ILE:HD11	2.15	0.56
1:B:28:ILE:HD11	1:B:89:ILE:HD12	1.87	0.56
1:E:63:ALA:HB2	1:E:72:GLN:HA	1.85	0.56
1:A:32:ASP:OD1	3:A:401:NAD:H1B	2.05	0.56
1:C:87:LEU:HB2	1:C:89:ILE:CD1	2.35	0.56
1:D:79:PRO:HA	1:D:82:LEU:CD1	2.35	0.56
1:H:3:VAL:HG13	1:H:27:ILE:HA	1.87	0.56
2:N:63:TYR:CE1	2:N:67:ASN:ND2	2.73	0.56
1:E:1:LEU:HD21	1:E:332:TRP:CE3	2.39	0.56
1:E:312:ASP:O	1:E:314:GLU:N	2.38	0.56
1:F:251:PHE:CE2	1:F:253:GLU:HB3	2.40	0.56
1:F:298:MET:HE2	1:F:306:LYS:HD3	1.87	0.56
1:G:131:GLY:N	1:G:134:ALA:HB2	2.17	0.56
1:G:213:ALA:HA	1:G:216:LEU:HD12	1.87	0.56
1:H:149:CYS:HA	1:H:317:TYR:HD1	1.69	0.56
1:Q:115:LYS:HG3	1:Q:142:PRO:O	2.05	0.56
1:C:271:LEU:HD12	1:C:272:ASP:N	2.20	0.56
1:C:84:TRP:CE3	1:C:84:TRP:HA	2.40	0.56
1:O:206:THR:HG23	1:O:229:ALA:HB3	1.86	0.56
1:O:323:ASP:O	1:O:327:ILE:HD13	2.05	0.56
1:A:74:VAL:HG23	1:A:75:SER:N	2.19	0.56
1:E:165:PHE:HD1	1:E:248:LYS:HD3	1.69	0.56
1:E:279:VAL:HG12	1:G:205:PRO:CD	2.36	0.56
1:G:130:VAL:HG23	1:G:320:ARG:HD3	1.86	0.56
1:H:18(A):TRP:HE1	1:H:23:SER:HB3	1.71	0.56
1:A:109:ILE:C	1:A:111:ALA:H	2.08	0.56
1:A:139:HIS:HB3	1:A:333:LYS:NZ	2.20	0.56
1:D:87:LEU:HD12	1:D:89:ILE:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:222:LYS:O	1:F:223:GLY:C	2.44	0.56
1:H:192:ASP:O	1:H:196:ALA:HB2	2.06	0.56
1:Q:260:ARG:HG2	1:Q:273:VAL:HG21	1.87	0.56
1:C:183:ARG:HG3	1:C:196:ALA:HA	1.87	0.56
1:C:289:SER:OG	1:C:320:ARG:HD2	2.05	0.56
1:E:226:ASN:HB3	1:G:300:MET:SD	2.46	0.56
1:F:126:PRO:CG	1:F:144:ILE:HG22	2.33	0.56
1:F:267:LEU:HB3	1:F:270:ILE:HB	1.88	0.56
1:H:130:VAL:HB	1:H:320:ARG:HD3	1.87	0.56
1:A:183:ARG:HE	1:A:187:ALA:HB3	1.70	0.56
1:B:279:VAL:HG11	1:D:204:VAL:HG13	1.87	0.56
1:E:18:CYS:HB3	1:E:319:GLN:OE1	2.05	0.56
1:F:144:ILE:C	1:F:144:ILE:HD12	2.27	0.56
1:H:162:ASP:O	1:H:166:GLY:N	2.38	0.56
1:D:7:GLY:HA3	1:D:96:THR:CG2	2.33	0.56
1:E:109:ILE:CA	1:E:113:ALA:HB3	2.35	0.56
1:E:3:VAL:HG22	1:E:91:ILE:CG2	2.36	0.56
1:F:296:LEU:HD22	1:H:228:ILE:HG21	1.88	0.56
1:H:266:GLU:HG2	1:H:267:LEU:HG	1.88	0.56
1:D:87:LEU:HD22	1:H:86:GLU:HB3	1.88	0.56
2:L:72:GLU:HG2	5:L:104:HOH:O	2.06	0.56
1:O:16:LEU:O	1:O:16:LEU:HD23	2.06	0.56
1:A:143:ILE:HD12	1:A:143:ILE:N	2.20	0.55
1:B:202:ASN:HD21	1:D:281:VAL:HG12	1.69	0.55
1:F:177:SER:HB3	1:F:234:THR:O	2.06	0.55
1:C:74:VAL:HG12	1:C:75:SER:H	1.71	0.55
1:F:92:VAL:O	1:F:116:VAL:HA	2.07	0.55
1:H:1:LEU:HD11	1:H:90:ASP:CB	2.32	0.55
2:K:74:ARG:C	1:O:181:ASP:OD1	2.45	0.55
1:A:28:ILE:HG22	1:A:69:LYS:NZ	2.21	0.55
1:B:162:ASP:HB2	1:B:167:ILE:HD12	1.88	0.55
1:D:215:ALA:CB	1:D:222:LYS:HA	2.35	0.55
1:F:7:GLY:O	1:F:9:GLY:N	2.37	0.55
1:G:251:PHE:CA	1:G:299:VAL:HG21	2.37	0.55
2:L:73:CYS:C	5:L:101:HOH:O	2.45	0.55
1:E:194:ARG:NH1	1:E:205:PRO:HB2	2.16	0.55
1:E:281:VAL:HG11	1:F:48:SER:OG	2.07	0.55
1:H:90:ASP:O	1:H:114:LYS:HB2	2.06	0.55
1:C:173:THR:HG23	1:C:228:ILE:HD11	1.89	0.55
1:C:251:PHE:CZ	1:C:254:GLU:HB2	2.41	0.55
1:D:168:ILE:HG12	1:D:246:VAL:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:67:ASN:O	2:N:73:CYS:SG	2.64	0.55
1:A:206:THR:HG21	1:A:231:ARG:HG2	1.87	0.55
1:B:281:VAL:CG1	1:D:202:ASN:HD21	2.20	0.55
1:D:15:PHE:CE1	1:D:322:VAL:HG22	2.42	0.55
1:D:3:VAL:O	1:D:27:ILE:HA	2.06	0.55
1:D:331:ASN:O	1:D:331:ASN:OD1	2.25	0.55
1:E:108:HIS:O	1:E:111:ALA:HB3	2.06	0.55
1:B:149:CYS:SG	2:J:78:ASN:CG	2.84	0.55
1:O:187:ALA:O	1:O:196:ALA:HB1	2.06	0.55
1:Q:14:ASN:ND2	1:Q:314:GLU:HB3	2.22	0.55
1:B:186:ASP:HB2	1:C:10:ARG:NH1	2.21	0.55
1:D:109:ILE:HA	1:D:113:ALA:O	2.07	0.55
1:D:154:LEU:HD21	1:D:172:MET:HG3	1.89	0.55
1:E:282:ASP:OD1	1:F:46:TYR:HB3	2.06	0.55
1:G:154:LEU:CD1	1:G:240:VAL:HG11	2.37	0.55
1:E:171:THR:CG2	1:G:306:LYS:HE3	2.36	0.55
1:F:167:ILE:HG21	1:F:221:LEU:CD1	2.36	0.55
1:F:270:ILE:HG23	1:F:289:SER:HB2	1.88	0.55
1:G:271:LEU:HD12	1:G:290:THR:O	2.06	0.55
1:H:72:GLN:N	1:H:72:GLN:NE2	2.55	0.55
1:H:188:SER:O	2:N:72:GLU:HB3	2.06	0.55
1:O:170:GLY:HA3	1:O:244:VAL:HG12	1.89	0.55
1:A:16:LEU:HD23	1:A:16:LEU:O	2.07	0.55
1:B:162:ASP:O	1:B:166:GLY:HA2	2.06	0.55
1:D:210:ALA:HA	1:D:213:ALA:HB3	1.89	0.55
1:F:202:ASN:CB	1:H:280:SER:OG	2.55	0.55
1:E:235:PRO:HB3	1:H:201:LEU:HD11	1.88	0.55
1:A:173:THR:HG23	1:A:228:ILE:CD1	2.37	0.55
1:B:172:MET:HG2	1:B:173:THR:N	2.22	0.55
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.89	0.55
1:C:70:ILE:HD13	1:C:70:ILE:C	2.26	0.55
1:E:299:VAL:HG13	1:E:304:MET:O	2.07	0.55
1:C:190:HIS:CB	1:C:196:ALA:HB2	2.37	0.54
1:D:191:ARG:NH1	2:I:61:GLU:HG2	2.22	0.54
1:D:332:TRP:HB3	5:D:519:HOH:O	2.08	0.54
1:F:14:ASN:HD22	1:F:314:GLU:HG2	1.70	0.54
1:F:222:LYS:O	1:F:222:LYS:HG3	2.07	0.54
1:F:298:MET:CE	1:F:306:LYS:HD3	2.36	0.54
1:G:193:LEU:H	1:G:193:LEU:HD22	1.72	0.54
2:M:57:SER:OG	2:M:60:LEU:HB3	2.06	0.54
1:O:28:ILE:HD11	1:O:89:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ALA:HB2	1:A:89:ILE:HD12	1.89	0.54
1:D:78:ASN:ND2	1:D:80:SER:HB2	2.15	0.54
1:Q:263:ALA:HB2	1:Q:271:LEU:HD23	1.88	0.54
1:E:79:PRO:HA	1:E:82:LEU:CD1	2.38	0.54
1:E:87:LEU:HB3	1:E:89:ILE:CD1	2.36	0.54
1:O:263:ALA:HB2	1:O:271:LEU:HD23	1.89	0.54
1:C:203:ILE:HG23	1:C:232:VAL:HG12	1.89	0.54
1:D:319:GLN:HE21	1:D:319:GLN:CA	2.21	0.54
1:E:181:ASP:HB2	4:E:402:SO4:O4	2.08	0.54
1:G:28:ILE:HD11	1:G:89:ILE:HD13	1.88	0.54
2:L:63:TYR:CZ	2:L:73:CYS:SG	3.01	0.54
1:A:293:ASP:CB	1:A:296:LEU:HD12	2.38	0.54
1:C:301:GLY:O	1:C:302:ASP:HB2	2.07	0.54
1:D:154:LEU:CD2	1:D:172:MET:HG3	2.38	0.54
1:D:157:PHE:CE1	1:D:242:LEU:HD23	2.43	0.54
1:F:107:LYS:HA	1:F:110:GLU:HG2	1.88	0.54
1:F:245:GLN:NE2	1:H:245:GLN:NE2	2.46	0.54
1:H:24:PRO:HB2	1:H:329:ALA:HB1	1.90	0.54
1:D:18:CYS:HB2	1:D:322:VAL:HG21	1.90	0.54
1:F:174:THR:HA	1:F:240:VAL:HA	1.88	0.54
1:H:218:LEU:HB3	1:H:221:LEU:HD23	1.89	0.54
1:O:233:PRO:HB2	1:Q:233:PRO:HB2	1.89	0.54
1:C:183:ARG:HH21	1:C:187:ALA:CB	2.20	0.54
1:C:214:VAL:CG1	1:C:218:LEU:HD12	2.38	0.54
1:E:176:HIS:ND1	1:E:231:ARG:NH1	2.56	0.54
1:E:178:TYR:HA	1:E:182:GLN:OE1	2.08	0.54
1:E:218:LEU:O	1:E:220:ASN:N	2.40	0.54
1:F:161:LEU:HB3	1:F:167:ILE:HD11	1.90	0.54
1:F:317:TYR:O	1:F:321:VAL:HG23	2.07	0.54
1:G:211:ALA:HB1	1:G:226:ASN:CA	2.32	0.54
1:B:255:VAL:O	1:B:258:ALA:HB3	2.08	0.54
1:D:198:ALA:HB1	1:D:201:LEU:HD21	1.88	0.54
1:D:327:ILE:O	1:D:331:ASN:HB3	2.08	0.54
1:E:133:ASN:HA	1:E:135:ASP:OD1	2.07	0.54
1:E:240:VAL:O	1:E:308:ILE:HA	2.08	0.54
1:G:162:ASP:O	1:G:166:GLY:N	2.36	0.54
1:O:139:HIS:HB3	1:O:333:LYS:NZ	2.22	0.54
1:O:17:ARG:NH1	1:O:53:PHE:HB2	2.22	0.54
1:C:14:ASN:HD22	1:C:14:ASN:N	2.06	0.54
1:A:39:GLN:HG2	1:D:188:SER:HB2	1.88	0.54
1:D:319:GLN:HE21	1:D:319:GLN:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:PHE:HB2	1:F:259:PHE:CE1	2.43	0.54
1:G:131:GLY:H	1:G:134:ALA:CB	2.17	0.54
1:G:232:VAL:O	1:G:234:THR:N	2.40	0.54
1:H:149:CYS:HA	1:H:317:TYR:CD1	2.43	0.54
1:B:202:ASN:ND2	1:D:281:VAL:HB	2.22	0.54
1:B:169:LYS:CD	1:D:301:GLY:HA3	2.38	0.54
1:D:323:ASP:C	1:D:325:ALA:N	2.61	0.54
1:A:188:SER:HB2	1:D:39:GLN:HE22	1.73	0.54
1:F:66:VAL:O	1:F:69:LYS:HG2	2.08	0.54
1:G:300:MET:CE	1:G:301:GLY:H	2.21	0.54
1:G:300:MET:HE3	1:G:301:GLY:H	1.72	0.54
2:L:63:TYR:CE2	2:L:72:GLU:HG3	2.43	0.54
1:C:330:ASN:ND2	1:C:330:ASN:N	2.54	0.53
1:D:1:LEU:HD23	1:D:91:ILE:CD1	2.38	0.53
1:E:133:ASN:N	1:E:133:ASN:ND2	2.56	0.53
1:E:269:GLY:HA2	1:E:288:PHE:CE1	2.44	0.53
1:F:139:HIS:HB2	1:F:331:ASN:OD1	2.08	0.53
1:G:226:ASN:ND2	1:G:227:GLY:H	2.06	0.53
1:H:81:LEU:O	1:H:82:LEU:C	2.46	0.53
2:L:60:LEU:HD22	2:L:63:TYR:CD2	2.43	0.53
1:B:0:LYS:HE2	1:B:25:LEU:O	2.09	0.53
1:C:29:ALA:HA	1:C:71:ILE:HG23	1.89	0.53
1:F:130:VAL:HG11	1:F:323:ASP:HB2	1.90	0.53
1:F:281:VAL:HG13	1:F:282:ASP:N	2.23	0.53
1:G:130:VAL:HA	1:G:134:ALA:CB	2.38	0.53
1:H:269:GLY:O	1:H:270:ILE:HD13	2.08	0.53
1:H:292:ILE:HD13	1:H:309:ALA:HB2	1.90	0.53
2:L:63:TYR:CE2	2:L:73:CYS:SG	3.01	0.53
1:O:84:TRP:CE3	1:O:84:TRP:HA	2.44	0.53
1:Q:129:VAL:H	1:Q:133:ASN:ND2	2.06	0.53
1:C:84:TRP:HE3	1:C:84:TRP:HA	1.73	0.53
1:D:167:ILE:HD12	1:D:221:LEU:HD11	1.91	0.53
1:E:182:GLN:HE22	1:E:231:ARG:HB3	1.74	0.53
1:E:3:VAL:HB	1:E:27:ILE:HD13	1.90	0.53
1:F:191:ARG:HG3	5:F:503:HOH:O	2.08	0.53
1:H:16:LEU:O	1:H:16:LEU:HD23	2.08	0.53
1:O:226:ASN:HB2	1:Q:300:MET:CE	2.38	0.53
1:E:20:ARG:HH22	1:E:322:VAL:HB	1.73	0.53
1:F:202:ASN:HB3	1:H:281:VAL:HG23	1.89	0.53
1:F:210:ALA:O	1:F:214:VAL:HG23	2.08	0.53
1:H:177:SER:HB3	1:H:235:PRO:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:ARG:NH1	1:H:195:ARG:HB2	2.23	0.53
2:K:69:GLU:HG2	1:O:77:ARG:NH2	2.23	0.53
1:Q:110:GLU:O	1:Q:112:GLY:N	2.42	0.53
1:Q:109:ILE:HA	1:Q:113:ALA:O	2.09	0.53
1:Q:187:ALA:O	1:Q:196:ALA:HB1	2.09	0.53
1:C:79:PRO:HB3	1:C:108:HIS:CE1	2.44	0.53
1:D:133:ASN:HD21	1:D:217:VAL:HA	1.73	0.53
1:F:21:LYS:H	1:F:21:LYS:CE	2.22	0.53
1:H:236:ASN:O	1:H:237:VAL:HB	2.08	0.53
1:A:256:ASN:O	1:A:260:ARG:HG3	2.08	0.53
1:C:173:THR:HG23	1:C:228:ILE:CD1	2.38	0.53
1:D:116:VAL:HG12	1:D:117:ILE:N	2.23	0.53
1:E:171:THR:HG23	1:G:306:LYS:HE3	1.91	0.53
1:E:280:SER:HB3	1:G:202:ASN:HB2	1.91	0.53
1:G:205:PRO:HB3	1:G:230:LEU:CD2	2.38	0.53
1:A:28:ILE:O	1:A:28:ILE:HG12	2.07	0.53
1:B:226:ASN:HD22	1:D:298:MET:CE	2.22	0.53
1:D:137:TYR:CZ	1:D:328:VAL:HG22	2.44	0.53
1:E:-1:ALA:O	1:E:0:LYS:HB2	2.07	0.53
1:F:262:SER:HA	1:F:266:GLU:HG3	1.90	0.53
1:F:277:PRO:CG	1:H:193:LEU:HD12	2.39	0.53
1:F:26:ASP:OD2	1:F:28:ILE:HD11	2.09	0.53
1:F:289:SER:HG	1:F:320:ARG:HD2	1.74	0.53
1:G:129:VAL:N	1:G:133:ASN:HD21	2.01	0.53
1:G:154:LEU:O	1:G:155:ALA:C	2.47	0.53
1:Q:100:VAL:HA	1:Q:118:ILE:HD13	1.89	0.53
1:A:129:VAL:HG23	1:A:217:VAL:HG11	1.90	0.53
1:A:86:GLU:CD	1:A:86:GLU:H	2.12	0.53
1:F:20:ARG:HB3	1:F:23:SER:OG	2.08	0.53
1:H:13:ARG:O	1:H:17:ARG:HG3	2.09	0.53
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.74	0.53
1:B:266:GLU:O	1:B:267:LEU:HD23	2.09	0.53
1:B:2:LYS:HB3	1:B:28:ILE:HD13	1.91	0.53
1:C:18(A):TRP:CD2	1:C:27:ILE:HD13	2.44	0.53
1:C:87:LEU:HB2	1:C:89:ILE:HD11	1.90	0.53
1:E:169:LYS:NZ	1:E:245:GLN:OE1	2.42	0.53
1:E:279:VAL:HB	1:G:203:ILE:O	2.08	0.53
1:H:66:VAL:O	1:H:68:GLY:N	2.41	0.53
2:M:70:THR:HG22	2:M:71:ASN:N	2.23	0.53
1:C:126:PRO:HG2	1:C:141:GLU:CG	2.39	0.53
1:E:279:VAL:CG1	1:G:204:VAL:HA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:THR:OG1	1:G:251:PHE:N	2.41	0.53
1:H:4:ALA:HB2	1:H:89:ILE:HD12	1.91	0.53
1:O:172:MET:HE1	1:O:211:ALA:HB2	1.90	0.53
1:A:1:LEU:HD22	1:A:329:ALA:HB2	1.91	0.52
1:B:190:HIS:ND1	1:B:191:ARG:N	2.58	0.52
1:B:173:THR:O	1:B:241:ASP:HB3	2.08	0.52
1:C:318:SER:O	1:C:322:VAL:HG23	2.09	0.52
1:E:79:PRO:HA	1:E:82:LEU:HG	1.91	0.52
1:H:271:LEU:HD12	1:H:272:ASP:H	1.74	0.52
1:H:42:HIS:C	1:H:43:LEU:HD23	2.29	0.52
1:O:298:MET:HE3	1:Q:226:ASN:HD22	1.74	0.52
1:B:27:ILE:HD12	1:B:27:ILE:N	2.25	0.52
1:D:174:THR:HB	1:D:240:VAL:HG12	1.91	0.52
1:E:171:THR:HA	1:E:226:ASN:O	2.09	0.52
1:F:130:VAL:HG22	1:F:324:LEU:HB2	1.92	0.52
1:F:131:GLY:H	1:F:134:ALA:HB2	1.75	0.52
1:G:312:ASP:HB3	1:G:316:GLY:H	1.75	0.52
1:H:4:ALA:CB	1:H:89:ILE:HD12	2.39	0.52
1:O:263:ALA:O	1:O:268:LYS:HA	2.09	0.52
1:Q:250:THR:OG1	1:Q:251:PHE:N	2.41	0.52
1:A:172:MET:HG2	1:A:173:THR:N	2.24	0.52
1:A:28:ILE:H	1:A:28:ILE:HD13	1.74	0.52
1:E:235:PRO:CG	1:E:284:ARG:NH2	2.72	0.52
1:F:32:ASP:HA	3:F:401:NAD:H2A	1.91	0.52
1:G:303:ASP:HB2	5:G:532:HOH:O	2.10	0.52
1:H:123:GLY:O	1:H:125:ILE:N	2.42	0.52
2:K:77:ASP:OD1	2:K:78:ASN:N	2.43	0.52
1:Q:110:GLU:C	1:Q:112:GLY:H	2.12	0.52
1:A:293:ASP:HB3	1:A:296:LEU:HD12	1.92	0.52
1:D:195:ARG:NH1	2:I:76:TYR:O	2.43	0.52
1:E:246:VAL:HG22	1:E:303:ASP:O	2.08	0.52
1:E:320:ARG:HA	1:E:320:ARG:NE	2.25	0.52
1:F:156:PRO:CB	1:F:290:THR:HG21	2.37	0.52
1:H:85:LYS:HB2	1:H:112:GLY:HA3	1.91	0.52
2:J:58:ASP:N	2:J:59:PRO:CD	2.73	0.52
1:B:253:GLU:HG3	4:B:402:SO4:O3	2.09	0.52
1:C:36:GLY:O	1:C:40:ALA:HB2	2.08	0.52
1:E:100:VAL:O	1:E:122(A):LYS:HB2	2.09	0.52
1:E:155:ALA:HB3	1:E:156:PRO:HD3	1.92	0.52
1:E:80:SER:HB3	1:E:107:LYS:HE2	1.91	0.52
1:F:17:ARG:NH2	1:F:53:PHE:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:LEU:HD13	1:G:271:LEU:CB	2.40	0.52
1:G:304:MET:HG2	1:G:304:MET:O	2.09	0.52
1:H:106:GLY:HA2	1:H:143:ILE:HD11	1.91	0.52
1:H:148:SER:HB2	5:N:110:HOH:O	2.09	0.52
1:H:66:VAL:C	1:H:68:GLY:N	2.63	0.52
1:Q:306:LYS:NZ	5:Q:526:HOH:O	2.38	0.52
1:B:256:ASN:HD21	1:B:297:THR:HG1	1.55	0.52
1:B:115:LYS:HD2	1:B:332:TRP:CZ3	2.44	0.52
1:D:249:LYS:HD2	1:D:302:ASP:CB	2.37	0.52
1:E:175:THR:HB	1:E:239:VAL:CG1	2.39	0.52
1:E:270:ILE:O	1:E:270:ILE:HG22	2.09	0.52
1:G:133:ASN:N	1:G:133:ASN:ND2	2.58	0.52
1:G:139:HIS:CD2	1:G:333:LYS:H	2.26	0.52
1:G:210:ALA:O	1:G:213:ALA:HB3	2.09	0.52
1:G:256:ASN:HA	1:G:259:PHE:CD2	2.45	0.52
1:H:215:ALA:HB1	1:H:222:LYS:CA	2.34	0.52
1:H:72:GLN:N	1:H:72:GLN:HE21	2.03	0.52
2:K:70:THR:OG1	2:K:73:CYS:SG	2.68	0.52
1:A:29:ALA:N	1:A:71:ILE:HG13	2.24	0.52
1:A:86:GLU:CD	1:A:86:GLU:N	2.63	0.52
1:H:314:GLU:HG2	3:H:401:NAD:H72N	1.74	0.52
2:L:58:ASP:N	2:L:59:PRO:CD	2.72	0.52
1:O:39:GLN:N	1:O:39:GLN:NE2	2.55	0.52
1:E:16:LEU:HD23	1:E:16:LEU:O	2.09	0.52
1:E:65:SER:HA	1:E:70:ILE:HA	1.92	0.52
1:E:28:ILE:CA	1:E:71:ILE:HD12	2.39	0.52
1:F:168:ILE:HD11	1:F:247:SER:HB3	1.92	0.52
1:G:18(A):TRP:HD1	1:G:25:LEU:HD12	1.75	0.52
1:H:183:ARG:HB2	1:H:196:ALA:O	2.09	0.52
1:O:281:VAL:HB	1:Q:202:ASN:HD21	1.73	0.52
1:C:183:ARG:CG	1:C:196:ALA:HA	2.40	0.52
1:D:252:ALA:N	1:D:299:VAL:HG21	2.25	0.52
1:E:3:VAL:HG11	1:E:93:ILE:HD11	1.92	0.52
1:G:85:LYS:N	1:G:112:GLY:HA3	2.25	0.52
1:O:280:SER:HB3	1:Q:203:ILE:HB	1.92	0.52
1:A:172:MET:HG2	1:A:173:THR:H	1.75	0.52
1:B:152:ASN:ND2	1:B:320:ARG:HG3	2.25	0.52
1:C:98:VAL:HG23	1:C:99:PHE:CE2	2.45	0.52
1:E:183:ARG:HA	1:E:183:ARG:HH11	1.75	0.52
1:F:37:VAL:HG13	1:F:64:ILE:CG2	2.39	0.52
1:G:239:VAL:HB	1:G:310:TRP:CE3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASP:OD2	1:A:195:ARG:NH1	2.43	0.51
1:A:70:ILE:HG22	1:A:71:ILE:N	2.25	0.51
1:C:266:GLU:HG2	1:C:267:LEU:N	2.25	0.51
1:E:194:ARG:HD3	1:E:205:PRO:HD2	1.91	0.51
1:E:19:GLY:O	1:E:20:ARG:O	2.28	0.51
1:E:195:ARG:NH2	1:E:231:ARG:HH21	2.08	0.51
1:F:248:LYS:HE3	5:F:524:HOH:O	2.09	0.51
1:G:330:ASN:C	1:G:331:ASN:HD22	2.14	0.51
1:Q:168:ILE:HD11	1:Q:247:SER:CB	2.39	0.51
1:B:16:LEU:HD23	1:B:16:LEU:O	2.09	0.51
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.45	0.51
1:E:133:ASN:H	1:E:133:ASN:HD22	1.55	0.51
1:E:289:SER:HB2	1:E:320:ARG:HH11	1.76	0.51
1:E:28:ILE:C	1:E:71:ILE:HG23	2.29	0.51
1:F:274:CYS:SG	1:F:275:ASP:N	2.84	0.51
1:F:300:MET:CE	1:H:169:LYS:HB2	2.40	0.51
1:A:30:ILE:HG12	1:A:71:ILE:HD11	1.92	0.51
1:B:234:THR:HG22	1:D:233:PRO:HG2	1.93	0.51
1:C:270:ILE:HD12	1:C:270:ILE:N	2.24	0.51
1:F:186:ASP:HA	1:F:196:ALA:O	2.10	0.51
1:F:190:HIS:ND1	1:F:192:ASP:N	2.56	0.51
1:F:61:GLU:HA	5:F:510:HOH:O	2.08	0.51
1:H:81:LEU:CD1	1:H:81:LEU:H	2.24	0.51
1:H:94:GLU:CD	1:H:99:PHE:HD2	2.14	0.51
1:B:133:ASN:HD22	1:B:133:ASN:H	1.58	0.51
1:D:320:ARG:HA	1:D:320:ARG:HE	1.74	0.51
1:E:166:GLY:O	1:E:246:VAL:HA	2.10	0.51
1:E:46:TYR:CD1	1:E:52:ILE:HG22	2.45	0.51
1:G:252:ALA:N	1:G:299:VAL:HG21	2.24	0.51
1:G:331:ASN:N	1:G:331:ASN:HD22	2.07	0.51
2:N:62:GLU:HG2	5:N:104:HOH:O	2.10	0.51
1:C:0:LYS:HB3	1:C:0:LYS:NZ	2.26	0.51
1:B:226:ASN:HB3	1:D:298:MET:CE	2.40	0.51
1:F:117:ILE:CB	1:F:144:ILE:HD11	2.41	0.51
1:F:228:ILE:HD13	1:F:228:ILE:H	1.75	0.51
1:G:294:SER:O	1:G:297:THR:HG22	2.11	0.51
1:H:85:LYS:O	1:H:87:LEU:N	2.37	0.51
1:O:31:ASN:HB2	1:O:74:VAL:HG22	1.92	0.51
1:Q:3:VAL:HG21	1:Q:25:LEU:HB3	1.91	0.51
1:A:228:ILE:C	1:A:228:ILE:HD12	2.31	0.51
1:B:292:ILE:HD12	1:B:307:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HA	1:B:320:ARG:NE	2.26	0.51
1:G:167:ILE:HG23	1:G:244:VAL:HB	1.93	0.51
1:E:205:PRO:HG3	1:G:310:TRP:HZ2	1.76	0.51
1:H:148:SER:OG	1:H:210:ALA:HB2	2.11	0.51
1:Q:171:THR:O	1:Q:242:LEU:HD12	2.10	0.51
1:A:128:TYR:CZ	1:A:137:TYR:HA	2.45	0.51
1:D:182:GLN:HE22	1:D:231:ARG:HB3	1.76	0.51
1:E:320:ARG:HA	1:E:320:ARG:HE	1.76	0.51
1:O:298:MET:HE1	1:Q:226:ASN:HB3	1.93	0.51
1:C:3:VAL:HG22	1:C:91:ILE:HG23	1.92	0.51
1:C:46:TYR:O	1:C:47:ASP:HB2	2.10	0.51
1:D:8:PHE:O	1:D:13:ARG:HG3	2.11	0.51
1:D:10:ARG:O	1:D:14:ASN:HB2	2.10	0.51
1:D:130:VAL:HG21	1:D:320:ARG:O	2.11	0.51
1:E:78:ASN:OD1	1:E:80:SER:HB3	2.10	0.51
1:G:294:SER:O	1:G:296:LEU:N	2.44	0.51
2:M:71:ASN:HA	2:M:74:ARG:NH1	2.26	0.51
1:E:120:ALA:O	1:E:145:SER:OG	2.29	0.51
1:E:131:GLY:HA3	1:E:270:ILE:HG21	1.93	0.51
1:G:6:ASN:ND2	1:G:31:ASN:HD22	2.09	0.51
1:H:25:LEU:HD21	1:H:325:ALA:HB1	1.93	0.51
1:B:87:LEU:HB2	1:B:89:ILE:CD1	2.41	0.51
1:E:109:ILE:HG23	1:E:116:VAL:HG23	1.92	0.51
1:E:5:ILE:HD13	1:E:5:ILE:C	2.30	0.51
1:F:3:VAL:HG12	1:F:4:ALA:N	2.25	0.51
1:G:251:PHE:HA	1:G:299:VAL:HG21	1.91	0.51
1:H:137:TYR:OH	1:H:328:VAL:HG13	2.11	0.51
1:F:226:ASN:ND2	1:H:298:MET:SD	2.83	0.51
2:N:73:CYS:O	2:N:74:ARG:C	2.49	0.51
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.76	0.51
1:Q:154:LEU:HA	1:Q:157:PHE:CE2	2.45	0.51
1:B:109:ILE:HA	1:B:113:ALA:O	2.11	0.50
1:B:134:ALA:HB1	1:B:327:ILE:HD13	1.93	0.50
1:D:265:LYS:HB2	1:D:266:GLU:OE1	2.11	0.50
1:D:20:ARG:HE	1:D:319:GLN:HE22	1.59	0.50
1:E:208:THR:HA	4:E:403:SO4:O1	2.11	0.50
1:F:172:MET:SD	1:F:172:MET:O	2.69	0.50
1:F:191:ARG:HG2	1:F:191:ARG:HH11	1.76	0.50
1:F:31:ASN:HA	1:F:74:VAL:O	2.12	0.50
1:G:208:THR:HG23	1:G:208:THR:O	2.10	0.50
1:H:157:PHE:HB2	1:H:259:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:LEU:C	1:O:16:LEU:HD23	2.30	0.50
1:A:101:ASP:CG	1:A:103:GLU:HB3	2.32	0.50
1:A:215:ALA:CB	1:A:222:LYS:HA	2.41	0.50
1:D:320:ARG:HA	1:D:320:ARG:NE	2.27	0.50
1:E:157:PHE:CE1	1:E:242:LEU:HD23	2.46	0.50
1:E:324:LEU:O	1:E:328:VAL:HG23	2.11	0.50
1:F:154:LEU:HD11	1:F:242:LEU:HD12	1.92	0.50
1:F:246:VAL:O	1:F:303:ASP:HB2	2.10	0.50
1:F:0:LYS:HZ3	1:F:24:PRO:HG3	1.76	0.50
1:G:184:LEU:O	1:G:185:LEU:HD23	2.10	0.50
1:E:280:SER:CB	1:G:203:ILE:H	2.23	0.50
1:D:86:GLU:HB3	1:H:28:ILE:HD11	1.94	0.50
1:O:169:LYS:HE2	1:Q:301:GLY:HA3	1.93	0.50
1:O:28:ILE:HD11	1:O:89:ILE:CD1	2.41	0.50
1:A:281:VAL:CB	1:C:202:ASN:HD21	2.24	0.50
1:F:139:HIS:CD2	1:F:333:LYS:HD2	2.47	0.50
1:F:325:ALA:O	1:F:328:VAL:HB	2.12	0.50
1:G:176:HIS:O	1:G:231:ARG:HA	2.11	0.50
1:H:108:HIS:HD2	1:H:116:VAL:HG11	1.76	0.50
1:H:44:LEU:O	1:H:53:PHE:HB2	2.10	0.50
1:O:301:GLY:HA3	1:Q:169:LYS:HD3	1.92	0.50
1:O:84:TRP:HE3	1:O:84:TRP:HA	1.75	0.50
1:A:82:LEU:HD13	1:A:84:TRP:CE2	2.46	0.50
1:A:98:VAL:HG23	1:A:99:PHE:N	2.27	0.50
1:C:250:THR:OG1	1:C:251:PHE:N	2.44	0.50
1:C:89:ILE:H	1:C:89:ILE:CD1	2.21	0.50
1:C:46:TYR:CE2	1:D:278:LEU:HD21	2.46	0.50
1:E:135:ASP:C	1:E:137:TYR:H	2.14	0.50
1:E:241:ASP:HA	1:E:308:ILE:HD13	1.92	0.50
1:E:281:VAL:HG21	1:F:48:SER:HA	1.93	0.50
1:G:179:THR:C	1:G:181:ASP:N	2.64	0.50
1:G:20:ARG:HH11	1:G:20:ARG:HG3	1.76	0.50
1:G:177:SER:OG	1:G:234:THR:HG22	2.11	0.50
1:H:162:ASP:HA	1:H:167:ILE:HG13	1.92	0.50
1:H:29:ALA:HA	1:H:71:ILE:HG23	1.94	0.50
1:H:242:LEU:O	1:H:306:LYS:HA	2.11	0.50
1:Q:170:GLY:HA3	1:Q:244:VAL:HG12	1.93	0.50
1:B:83:PRO:HG2	1:B:87:LEU:CD1	2.41	0.50
1:D:4:ALA:HB2	1:D:89:ILE:HG12	1.93	0.50
1:D:64:ILE:HG23	1:D:73:VAL:CG2	2.41	0.50
1:G:132:VAL:HG12	1:G:133:ASN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:GLN:HA	1:H:195:ARG:O	2.12	0.50
1:H:31:ASN:OD1	1:H:75:SER:HA	2.12	0.50
1:H:83:PRO:HB2	1:H:86:GLU:CG	2.41	0.50
1:Q:206:THR:HG22	1:Q:229:ALA:HB3	1.93	0.50
1:D:146:ASN:HD22	1:D:321:VAL:HG23	1.76	0.50
1:E:170:GLY:HA3	1:E:244:VAL:HG12	1.92	0.50
1:E:198:ALA:HB3	1:E:201:LEU:HD11	1.92	0.50
1:E:157:PHE:CE1	1:E:307:VAL:HB	2.46	0.50
1:F:202:ASN:HB2	1:H:280:SER:OG	2.12	0.50
1:F:32:ASP:O	1:F:75:SER:HB2	2.12	0.50
1:G:1:LEU:HD13	1:G:329:ALA:HB1	1.94	0.50
1:Q:28:ILE:C	1:Q:28:ILE:HD12	2.31	0.50
1:A:139:HIS:CE1	1:A:333:LYS:H	2.29	0.50
1:D:162:ASP:O	1:D:166:GLY:HA2	2.12	0.50
1:E:174:THR:O	1:E:174:THR:HG23	2.11	0.50
1:F:284:ARG:HA	1:F:312:ASP:OD2	2.11	0.50
1:H:183:ARG:O	1:H:198:ALA:HA	2.11	0.50
1:H:195:ARG:HG2	1:H:195:ARG:O	2.11	0.50
1:O:266:GLU:HG2	1:O:267:LEU:HG	1.94	0.50
1:A:146:ASN:ND2	1:A:321:VAL:HG22	2.27	0.50
1:A:37:VAL:CG2	1:A:63:ALA:N	2.75	0.50
1:D:288:PHE:N	1:D:288:PHE:CD1	2.80	0.50
1:E:114:LYS:HD2	1:E:332:TRP:HZ2	1.76	0.50
1:E:-1:ALA:N	5:E:514:HOH:O	2.43	0.50
1:E:85:LYS:HB2	1:E:112:GLY:HA3	1.93	0.50
1:F:5:ILE:CB	1:F:30:ILE:HG23	2.34	0.50
1:F:89:ILE:O	1:F:113:ALA:HA	2.12	0.50
1:G:173:THR:HG23	1:G:228:ILE:CD1	2.42	0.50
1:H:317:TYR:O	1:H:320:ARG:HB2	2.11	0.50
1:O:281:VAL:CG2	1:Q:202:ASN:HD21	2.24	0.50
1:D:178:TYR:HA	1:D:231:ARG:HD2	1.93	0.50
1:D:62:THR:CG2	1:H:74:VAL:HG22	2.42	0.50
1:E:176:HIS:O	1:E:231:ARG:HA	2.12	0.50
1:E:330:ASN:HB3	5:E:540:HOH:O	2.11	0.50
1:E:9:GLY:HA3	3:E:401:NAD:O5B	2.12	0.50
1:F:31:ASN:ND2	5:F:502:HOH:O	2.44	0.50
2:L:60:LEU:HD22	2:L:63:TYR:HD2	1.77	0.50
1:A:266:GLU:HG2	1:A:267:LEU:N	2.26	0.49
1:B:134:ALA:HB1	1:B:327:ILE:CD1	2.42	0.49
1:B:279:VAL:HG21	1:D:197:ARG:HG3	1.93	0.49
1:F:165:PHE:CE1	1:F:250:THR:HB	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ASP:CB	1:F:67:ASP:H	2.23	0.49
1:G:165:PHE:O	1:G:246:VAL:HB	2.11	0.49
1:G:84:TRP:CE3	1:G:89:ILE:HG13	2.47	0.49
1:H:156:PRO:HB2	1:H:290:THR:HG21	1.94	0.49
1:H:314:GLU:HG2	3:H:401:NAD:N7N	2.27	0.49
1:E:183:ARG:NH2	2:N:74:ARG:HH22	2.10	0.49
1:O:281:VAL:H	1:Q:202:ASN:ND2	2.06	0.49
1:Q:194:ARG:HD3	1:Q:205:PRO:O	2.12	0.49
1:D:118:ILE:HG22	1:D:118:ILE:O	2.10	0.49
1:F:23:SER:O	1:F:25:LEU:N	2.41	0.49
1:H:20:ARG:HG3	1:H:20:ARG:HH11	1.77	0.49
1:H:221:LEU:N	1:H:221:LEU:HD22	2.27	0.49
1:F:300:MET:HG2	1:H:226:ASN:OD1	2.13	0.49
2:K:58:ASP:CG	2:K:61:GLU:HG3	2.32	0.49
1:E:146:ASN:HD22	1:E:324:LEU:HD22	1.77	0.49
1:E:176:HIS:CE1	1:E:231:ARG:NH1	2.81	0.49
1:F:109:ILE:C	1:F:111:ALA:H	2.15	0.49
1:F:260:ARG:HA	1:F:263:ALA:HB3	1.93	0.49
1:E:197:ARG:NH1	1:G:282:ASP:OD2	2.46	0.49
1:H:176:HIS:CE1	1:H:238:SER:HG	2.30	0.49
1:H:11:ILE:HD11	3:H:401:NAD:C3N	2.42	0.49
1:H:84:TRP:HB3	1:H:89:ILE:HG21	1.94	0.49
1:Q:61:GLU:HG3	5:Q:561:HOH:O	2.13	0.49
1:B:162:ASP:OD1	1:B:167:ILE:N	2.46	0.49
1:B:284:ARG:O	1:B:285:CYS:HB2	2.11	0.49
1:A:282:ASP:HA	1:B:52:ILE:HD11	1.92	0.49
1:C:236:ASN:HD21	1:C:312:ASP:CG	2.16	0.49
1:C:281:VAL:C	1:C:283:PHE:H	2.14	0.49
1:D:109:ILE:HG22	1:D:113:ALA:O	2.12	0.49
1:D:168:ILE:O	1:D:224:LYS:HD3	2.13	0.49
1:E:94:GLU:OE2	1:E:99:PHE:HB2	2.13	0.49
1:F:173:THR:HG23	1:F:228:ILE:HD11	1.94	0.49
1:G:256:ASN:ND2	1:G:256:ASN:H	2.10	0.49
1:O:218:LEU:HB3	1:O:221:LEU:HD23	1.95	0.49
1:O:31:ASN:HA	1:O:74:VAL:O	2.13	0.49
1:Q:127:THR:N	4:Q:404:SO4:O3	2.45	0.49
1:A:281:VAL:HB	1:C:202:ASN:HD21	1.77	0.49
1:C:197:ARG:HH11	1:C:197:ARG:HG3	1.76	0.49
1:C:214:VAL:O	1:C:218:LEU:HB2	2.12	0.49
1:E:85:LYS:N	1:E:112:GLY:HA3	2.27	0.49
1:G:28:ILE:N	1:G:28:ILE:HD13	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:THR:HG21	1:O:77:ARG:HE	1.77	0.49
1:O:202:ASN:ND2	1:Q:281:VAL:H	2.11	0.49
1:A:171:THR:CG2	1:C:306:LYS:HZ3	2.25	0.49
1:A:293:ASP:CG	1:A:296:LEU:HD12	2.32	0.49
1:C:157:PHE:HB2	1:C:259:PHE:CE1	2.48	0.49
1:D:16:LEU:HD23	1:D:16:LEU:C	2.33	0.49
1:E:157:PHE:HB2	1:E:259:PHE:CZ	2.48	0.49
2:I:69:GLU:OE2	2:I:69:GLU:N	2.40	0.49
1:Q:204:VAL:HB	1:Q:231:ARG:HB2	1.95	0.49
1:A:183:ARG:NE	1:A:187:ALA:HB3	2.28	0.49
1:B:53:PHE:CE2	1:B:55:ALA:HB3	2.48	0.49
1:C:133:ASN:C	1:C:135:ASP:N	2.66	0.49
1:B:279:VAL:HG22	1:D:197:ARG:HG3	1.95	0.49
1:D:83:PRO:HB3	1:H:72:GLN:OE1	2.12	0.49
1:E:132:VAL:HG11	1:E:217:VAL:CG2	2.43	0.49
1:E:38:LYS:HB2	1:E:39:GLN:HE22	1.77	0.49
1:F:128:TYR:HA	1:F:133:ASN:HD21	1.77	0.49
1:H:154:LEU:O	1:H:158:VAL:HG23	2.13	0.49
1:F:300:MET:HG2	1:H:226:ASN:HD21	1.77	0.49
1:Q:157:PHE:HB2	1:Q:259:PHE:CE1	2.47	0.49
1:B:117:ILE:C	1:B:117:ILE:HD13	2.32	0.49
1:C:271:LEU:HA	1:C:290:THR:O	2.13	0.49
1:D:124:ASP:O	1:D:125:ILE:CB	2.61	0.49
1:B:194:ARG:NH2	1:D:277:PRO:HA	2.27	0.49
1:H:96:THR:OG1	1:H:98:VAL:HG22	2.11	0.49
1:A:109:ILE:HA	1:A:113:ALA:O	2.13	0.49
1:B:102:ARG:HG2	1:B:102:ARG:NH1	2.28	0.49
1:B:192:ASP:OD1	1:B:194:ARG:HB2	2.12	0.49
1:D:142:PRO:O	1:D:143:ILE:HD12	2.13	0.49
1:E:118:ILE:HD12	1:E:118:ILE:H	1.77	0.49
1:E:1:LEU:HD22	1:E:329:ALA:HA	1.94	0.49
1:E:204:VAL:HA	1:E:205:PRO:HD3	1.70	0.49
1:F:211:ALA:HB1	1:F:226:ASN:HA	1.95	0.49
2:K:71:ASN:HB3	1:O:183:ARG:CZ	2.43	0.49
1:O:194:ARG:HD2	1:O:205:PRO:O	2.12	0.49
1:A:130:VAL:HG23	5:A:503:HOH:O	2.12	0.49
1:A:192:ASP:HA	5:A:509:HOH:O	2.11	0.49
1:B:292:ILE:HD12	1:B:307:VAL:CG1	2.43	0.49
1:D:11:ILE:HD11	3:D:401:NAD:C2N	2.42	0.49
1:E:175:THR:HB	1:E:239:VAL:HG12	1.95	0.49
1:G:18(A):TRP:CH2	1:G:69:LYS:HE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:ASN:HB2	1:G:74:VAL:HG22	1.95	0.49
2:J:58:ASP:HA	2:J:61:GLU:HG3	1.94	0.49
2:M:58:ASP:H	2:M:59:PRO:CD	2.26	0.49
1:Q:98:VAL:HG23	1:Q:99:PHE:CE2	2.48	0.49
1:B:39:GLN:OE1	1:C:188:SER:HB2	2.13	0.48
1:B:226:ASN:HB3	1:D:298:MET:HE1	1.93	0.48
1:E:154:LEU:HD11	1:E:172:MET:HG3	1.95	0.48
1:E:38:LYS:HB2	1:E:39:GLN:NE2	2.27	0.48
1:E:63:ALA:HB1	1:E:72:GLN:HA	1.94	0.48
1:F:178:TYR:HD1	1:F:178:TYR:O	1.96	0.48
1:F:260:ARG:HB3	1:F:264:GLU:OE2	2.13	0.48
2:K:69:GLU:HB3	1:O:98:VAL:CG1	2.33	0.48
1:O:26:ASP:O	1:O:28:ILE:HG23	2.12	0.48
1:B:177:SER:CB	1:B:234:THR:O	2.61	0.48
1:C:74:VAL:HG12	1:C:75:SER:N	2.28	0.48
1:D:203:ILE:HG12	1:D:232:VAL:HG12	1.95	0.48
1:D:215:ALA:HB3	5:D:539:HOH:O	2.13	0.48
1:D:232:VAL:O	1:D:234:THR:N	2.44	0.48
1:D:169:LYS:NZ	1:D:245:GLN:NE2	2.61	0.48
1:F:114:LYS:N	1:F:114:LYS:CD	2.74	0.48
1:F:56:ASP:HB2	1:F:67:ASP:CA	2.43	0.48
1:H:64:ILE:HG13	1:H:64:ILE:O	2.13	0.48
1:H:8:PHE:CE1	1:H:16:LEU:HD12	2.49	0.48
1:O:17:ARG:HD2	1:O:53:PHE:CE1	2.48	0.48
1:O:58:LYS:C	1:O:58:LYS:HD3	2.34	0.48
1:Q:251:PHE:CZ	1:Q:254:GLU:HB2	2.48	0.48
1:A:13:ARG:NE	1:A:43:LEU:HB3	2.29	0.48
1:C:258:ALA:HA	1:C:261:ASP:OD2	2.13	0.48
1:D:172:MET:CG	1:D:173:THR:N	2.77	0.48
1:E:315:TRP:O	1:E:318:SER:HB2	2.13	0.48
1:F:238:SER:HB2	1:F:311:TYR:CZ	2.48	0.48
1:F:52:ILE:HD12	1:F:52:ILE:N	2.28	0.48
1:G:18(A):TRP:CD1	1:G:25:LEU:HD12	2.48	0.48
1:F:235:PRO:HB3	1:G:201:LEU:HD11	1.94	0.48
1:G:293:ASP:HB3	1:G:296:LEU:CD1	2.39	0.48
1:H:86:GLU:CD	1:H:86:GLU:N	2.64	0.48
1:O:27:ILE:CD1	1:O:27:ILE:N	2.76	0.48
1:A:101:ASP:O	1:A:102:ARG:C	2.52	0.48
1:B:4:ALA:HA	1:B:29:ALA:O	2.13	0.48
1:C:213:ALA:O	1:C:216:LEU:HB2	2.14	0.48
1:D:245:GLN:HG2	1:D:303:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ASN:O	1:H:298:MET:HE3	2.13	0.48
1:F:9:GLY:HA3	3:F:401:NAD:O5B	2.13	0.48
1:H:79:PRO:HG3	1:H:99:PHE:CZ	2.49	0.48
1:Q:115:LYS:HE2	1:Q:141:GLU:O	2.14	0.48
1:Q:132:VAL:HG21	1:Q:155:ALA:HB1	1.95	0.48
1:B:149:CYS:SG	2:J:78:ASN:ND2	2.86	0.48
1:B:36:GLY:HA3	1:B:38:LYS:HE3	1.95	0.48
1:D:231:ARG:HH21	2:I:78:ASN:C	2.17	0.48
1:E:78:ASN:OD1	1:E:107:LYS:HE2	2.13	0.48
1:H:20:ARG:NH1	1:H:20:ARG:HG3	2.28	0.48
2:N:62:GLU:O	2:N:65:LYS:HB3	2.13	0.48
1:Q:242:LEU:HD12	1:Q:243:VAL:H	1.78	0.48
1:C:146:ASN:O	1:C:147:ALA:HB3	2.13	0.48
1:D:143:ILE:O	1:D:143:ILE:HG22	2.13	0.48
1:G:197:ARG:HG3	1:G:197:ARG:HH11	1.79	0.48
1:O:176:HIS:HB3	1:O:231:ARG:HD3	1.96	0.48
1:Q:28:ILE:HD12	1:Q:29:ALA:HB2	1.96	0.48
1:B:195:ARG:HH12	2:J:76:TYR:H	1.62	0.48
1:B:251:PHE:CE2	1:B:253:GLU:HB2	2.49	0.48
1:B:307:VAL:HG12	1:B:308:ILE:N	2.28	0.48
1:B:52:ILE:N	1:B:52:ILE:HD12	2.29	0.48
1:C:126:PRO:HD2	1:C:143:ILE:O	2.14	0.48
1:C:27:ILE:CG2	1:C:71:ILE:HD13	2.43	0.48
1:D:21:LYS:O	1:D:22:ASP:HB2	2.13	0.48
1:F:52:ILE:CD1	1:F:52:ILE:H	2.27	0.48
1:G:20:ARG:NH1	1:G:20:ARG:HG3	2.29	0.48
1:H:164:LYS:H	1:H:164:LYS:CD	2.26	0.48
1:H:81:LEU:HD12	1:H:81:LEU:N	2.29	0.48
1:A:87:LEU:HB2	1:A:89:ILE:HG12	1.96	0.48
1:B:27:ILE:CD1	1:B:27:ILE:N	2.77	0.48
1:E:10:ARG:HB2	3:E:401:NAD:O1N	2.13	0.48
1:F:306:LYS:NZ	1:H:173:THR:OG1	2.28	0.48
2:I:71:ASN:HA	2:I:74:ARG:NH2	2.28	0.48
1:O:298:MET:HE3	1:Q:226:ASN:ND2	2.29	0.48
1:Q:37:VAL:HG22	1:Q:73:VAL:HB	1.96	0.48
1:A:139:HIS:CD2	1:A:333:LYS:HE2	2.48	0.48
1:A:202:ASN:O	1:A:233:PRO:HD3	2.13	0.48
1:B:220:ASN:HD22	1:B:220:ASN:C	2.17	0.48
1:C:91:ILE:HD11	1:C:93:ILE:CD1	2.43	0.48
1:D:117:ILE:HA	1:D:144:ILE:HG13	1.96	0.48
1:D:260:ARG:O	1:D:263:ALA:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:PHE:HE2	1:F:253:GLU:HB3	1.79	0.48
1:G:181:ASP:OD2	2:M:75:THR:HA	2.14	0.48
1:H:11:ILE:HD11	3:H:401:NAD:H71N	1.79	0.48
1:H:288:PHE:C	1:H:290:THR:N	2.67	0.48
1:Q:16:LEU:O	1:Q:16:LEU:HD12	2.14	0.48
1:O:281:VAL:CB	1:Q:202:ASN:HD21	2.27	0.48
1:Q:31:ASN:OD1	1:Q:74:VAL:HG22	2.14	0.48
1:A:78:ASN:HD22	1:A:81:LEU:CD1	2.26	0.48
1:B:14:ASN:OD1	1:B:50:LEU:HD11	2.14	0.48
1:E:281:VAL:O	1:E:281:VAL:HG22	2.14	0.48
1:H:42:HIS:O	1:H:43:LEU:HD23	2.14	0.48
1:O:18(A):TRP:CE2	1:O:27:ILE:HD13	2.48	0.48
1:A:194:ARG:HD3	1:C:278:LEU:O	2.14	0.47
1:C:29:ALA:HA	1:C:71:ILE:CG2	2.43	0.47
1:D:122:GLY:HA3	1:D:125:ILE:HG21	1.95	0.47
1:E:22:ASP:HA	5:E:514:HOH:O	2.14	0.47
1:F:85:LYS:HE2	1:F:112:GLY:HA2	1.94	0.47
1:G:162:ASP:HA	1:G:167:ILE:HG12	1.96	0.47
1:G:252:ALA:HB1	1:G:297:THR:HG23	1.94	0.47
2:N:60:LEU:HD11	2:N:72:GLU:HB2	1.96	0.47
1:D:270:ILE:HD12	1:D:270:ILE:N	2.29	0.47
1:E:172:MET:HA	1:E:241:ASP:O	2.14	0.47
1:E:279:VAL:HG12	1:G:204:VAL:HA	1.95	0.47
1:G:133:ASN:H	1:G:133:ASN:ND2	2.12	0.47
1:G:-1:ALA:CB	1:G:26:ASP:HB2	2.43	0.47
1:G:271:LEU:CD1	1:G:290:THR:O	2.61	0.47
1:H:84:TRP:CG	1:H:89:ILE:HG21	2.49	0.47
1:A:142:PRO:C	1:A:143:ILE:HD12	2.34	0.47
1:C:48:SER:HA	1:D:281:VAL:HG11	1.96	0.47
1:D:62:THR:CB	1:H:74:VAL:HG22	2.45	0.47
1:E:274:CYS:SG	1:E:276:GLU:HB2	2.54	0.47
1:E:5:ILE:O	1:E:5:ILE:HG23	2.13	0.47
1:G:166:GLY:O	1:G:246:VAL:HA	2.13	0.47
1:H:133:ASN:OD1	1:H:217:VAL:HG12	2.14	0.47
1:C:9:GLY:O	1:C:13:ARG:HG3	2.14	0.47
1:A:280:SER:HG	1:C:203:ILE:H	1.60	0.47
1:E:158:VAL:HG11	1:E:225:LEU:HD11	1.95	0.47
1:F:38:LYS:CE	1:G:193:LEU:HD21	2.44	0.47
1:F:300:MET:HE3	1:H:169:LYS:HD2	1.96	0.47
1:F:279:VAL:HG11	1:H:204:VAL:HG22	1.95	0.47
1:E:193:LEU:HD21	1:H:39:GLN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ASP:HB3	1:H:51:GLY:H	1.79	0.47
2:M:75:THR:C	2:M:76:TYR:HD1	2.18	0.47
2:L:71:ASN:HB2	1:Q:183:ARG:CZ	2.45	0.47
1:A:156:PRO:HB2	1:A:290:THR:CG2	2.41	0.47
1:A:17:ARG:CZ	1:A:53:PHE:HB2	2.44	0.47
1:B:68:GLY:O	1:B:70:ILE:HD12	2.14	0.47
1:D:231:ARG:HH11	1:D:231:ARG:HG3	1.79	0.47
1:B:171:THR:CG2	1:D:306:LYS:HE3	2.44	0.47
1:D:11:ILE:HD11	3:D:401:NAD:N1N	2.29	0.47
1:E:151:THR:HG23	1:E:214:VAL:HG22	1.97	0.47
1:E:218:LEU:C	1:E:220:ASN:H	2.18	0.47
1:F:222:LYS:O	1:F:224:LYS:N	2.47	0.47
1:F:303:ASP:OD1	1:H:169:LYS:NZ	2.48	0.47
1:G:186:ASP:HA	1:G:196:ALA:O	2.14	0.47
1:G:271:LEU:CD1	1:G:292:ILE:HD13	2.29	0.47
1:H:119:THR:O	1:H:120:ALA:HB2	2.14	0.47
2:N:60:LEU:HD23	2:N:60:LEU:C	2.33	0.47
1:O:85:LYS:HB3	1:O:86:GLU:OE1	2.15	0.47
1:B:252:ALA:O	1:B:255:VAL:N	2.47	0.47
1:C:126:PRO:HG2	1:C:141:GLU:HG3	1.96	0.47
1:C:280:SER:HA	1:C:310:TRP:CZ3	2.49	0.47
1:C:324:LEU:O	1:C:328:VAL:HG23	2.15	0.47
1:D:192:ASP:OD2	1:D:195:ARG:HG3	2.14	0.47
1:F:287:ASP:OD1	1:F:319:GLN:NE2	2.37	0.47
1:F:315:TRP:O	1:F:319:GLN:HG2	2.15	0.47
1:F:66:VAL:O	1:F:67:ASP:HB2	2.14	0.47
1:G:123:GLY:O	1:G:125:ILE:N	2.45	0.47
1:H:164:LYS:N	1:H:164:LYS:CD	2.74	0.47
2:K:73:CYS:O	2:K:74:ARG:C	2.52	0.47
1:H:181:ASP:OD1	2:N:76:TYR:CG	2.68	0.47
1:O:320:ARG:NE	1:O:320:ARG:HA	2.29	0.47
1:A:78:ASN:HD22	1:A:81:LEU:HD11	1.80	0.47
1:B:149:CYS:HG	2:J:78:ASN:CG	2.16	0.47
1:C:64:ILE:HG23	1:C:73:VAL:HG21	1.97	0.47
1:D:288:PHE:C	1:D:290:THR:H	2.17	0.47
1:D:57:VAL:O	1:D:57:VAL:HG12	2.14	0.47
1:G:221:LEU:HD21	1:G:225:LEU:CD1	2.44	0.47
1:G:96:THR:OG1	1:G:98:VAL:HG22	2.15	0.47
1:B:326:ASP:O	1:B:330:ASN:OD1	2.33	0.47
1:E:138:SER:C	1:E:140:ASP:H	2.18	0.47
1:E:161:LEU:HD13	1:E:244:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:GLU:OE2	1:E:276:GLU:HA	2.15	0.47
1:F:225:LEU:O	1:F:226:ASN:HB2	2.14	0.47
1:G:208:THR:C	1:G:210:ALA:H	2.18	0.47
1:H:250:THR:OG1	1:H:251:PHE:N	2.47	0.47
1:H:84:TRP:CE3	1:H:89:ILE:HG13	2.49	0.47
2:K:76:TYR:H	1:O:181:ASP:CG	2.17	0.47
1:A:76:ASN:HD22	1:A:76:ASN:C	2.16	0.47
1:C:177:SER:CB	1:C:234:THR:O	2.59	0.47
1:D:105:ALA:O	1:D:108:HIS:HB2	2.15	0.47
1:D:130:VAL:HB	1:D:320:ARG:HD3	1.97	0.47
1:E:80:SER:HB2	1:E:107:LYS:CG	2.45	0.47
1:E:272:ASP:HB2	1:E:288:PHE:CG	2.50	0.47
1:E:10:ARG:N	3:E:401:NAD:O2A	2.44	0.47
1:H:1:LEU:CD1	1:H:90:ASP:CB	2.92	0.47
1:O:281:VAL:CG2	1:Q:202:ASN:ND2	2.75	0.47
1:Q:168:ILE:CD1	1:Q:247:SER:HB3	2.43	0.47
1:Q:289:SER:C	1:Q:290:THR:HG22	2.35	0.47
1:A:62:THR:O	1:A:62:THR:HG23	2.15	0.47
1:C:84:TRP:HB3	1:C:113:ALA:H	1.79	0.47
1:F:109:ILE:H	1:F:109:ILE:HD12	1.79	0.47
1:F:236:ASN:O	1:F:237:VAL:HB	2.14	0.47
1:F:55:ALA:HB1	1:F:67:ASP:OD1	2.15	0.47
1:H:78:ASN:CG	1:H:81:LEU:HD13	2.35	0.47
1:O:172:MET:HE3	1:O:211:ALA:HB2	1.97	0.47
1:A:255:VAL:HG12	1:A:259:PHE:CE2	2.50	0.47
1:B:128:TYR:HE1	1:B:136:ALA:HB3	1.80	0.47
1:C:183:ARG:HH21	1:C:187:ALA:HB1	1.79	0.47
1:C:194:ARG:O	1:C:197:ARG:HG2	2.15	0.47
1:D:271:LEU:C	1:D:271:LEU:HD23	2.36	0.47
1:H:88:GLY:O	1:H:89:ILE:C	2.53	0.47
1:D:150:THR:H	2:I:78:ASN:ND2	2.13	0.47
1:O:79:PRO:HB2	1:O:107:LYS:HB2	1.96	0.47
1:B:236:ASN:C	1:B:237:VAL:HG23	2.35	0.46
1:B:251:PHE:CZ	1:B:254:GLU:HB2	2.50	0.46
1:C:191:ARG:HB2	1:C:191:ARG:HH11	1.80	0.46
1:E:250:THR:HA	1:E:254:GLU:OE1	2.15	0.46
1:E:37:VAL:O	1:E:41:SER:HB2	2.14	0.46
1:F:149:CYS:HB3	3:F:401:NAD:C5N	2.40	0.46
1:F:205:PRO:HA	1:F:230:LEU:HD23	1.97	0.46
1:F:277:PRO:HA	1:H:194:ARG:NE	2.30	0.46
1:O:115:LYS:HG3	1:O:142:PRO:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:137:TYR:HE2	5:Q:527:HOH:O	1.98	0.46
1:A:279:VAL:CG1	1:C:204:VAL:HG22	2.44	0.46
1:A:28:ILE:N	1:A:28:ILE:HD13	2.31	0.46
1:B:168:ILE:HD11	1:B:247:SER:OG	2.14	0.46
1:B:307:VAL:CG1	1:B:308:ILE:N	2.79	0.46
1:B:45:LYS:NZ	1:B:55:ALA:O	2.48	0.46
1:C:146:ASN:HB3	1:C:317:TYR:OH	2.15	0.46
1:C:208:THR:HG22	1:C:228:ILE:HA	1.97	0.46
1:D:169:LYS:NZ	1:D:245:GLN:HE22	2.12	0.46
1:E:2:LYS:O	1:E:90:ASP:HB2	2.15	0.46
1:E:58:LYS:HG3	5:E:503:HOH:O	2.14	0.46
1:F:126:PRO:HG2	1:F:144:ILE:HA	1.97	0.46
1:G:38:LYS:HG3	1:G:39:GLN:N	2.30	0.46
1:G:37:VAL:HG13	1:G:73:VAL:CG1	2.45	0.46
1:G:79:PRO:O	1:G:111:ALA:HB2	2.15	0.46
1:A:0:LYS:H3	1:A:0:LYS:CE	2.25	0.46
1:A:200:ALA:C	1:A:201:LEU:HG	2.36	0.46
1:A:272:ASP:O	1:A:291:THR:HA	2.16	0.46
1:D:106:GLY:C	1:D:108:HIS:N	2.68	0.46
1:D:154:LEU:HD22	1:D:172:MET:HE2	1.97	0.46
1:F:0:LYS:HZ2	1:F:24:PRO:HG3	1.78	0.46
1:F:13:ARG:HH11	1:F:13:ARG:HG3	1.79	0.46
1:F:256:ASN:HD21	1:F:297:THR:CB	2.28	0.46
1:F:27:ILE:N	1:F:27:ILE:CD1	2.78	0.46
1:F:243:VAL:HG22	1:F:306:LYS:HG3	1.96	0.46
1:H:139:HIS:HE1	1:H:332:TRP:CE3	2.34	0.46
1:H:266:GLU:HG2	1:H:267:LEU:N	2.29	0.46
1:A:176:HIS:HB3	1:A:231:ARG:HD3	1.98	0.46
1:E:-1:ALA:HB1	1:E:26:ASP:HB2	1.96	0.46
1:F:166:GLY:O	1:F:246:VAL:HA	2.15	0.46
1:O:183:ARG:HG2	1:O:196:ALA:HA	1.98	0.46
1:B:277:PRO:CB	1:D:194:ARG:HE	2.28	0.46
1:E:236:ASN:CG	1:E:237:VAL:H	2.19	0.46
1:E:279:VAL:HG11	1:G:204:VAL:HG13	1.96	0.46
1:G:194:ARG:HD3	1:G:205:PRO:O	2.15	0.46
1:C:0:LYS:HG2	1:C:0:LYS:O	2.16	0.46
1:D:204:VAL:HA	1:D:205:PRO:HD3	1.74	0.46
1:E:139:HIS:CG	1:E:139:HIS:O	2.68	0.46
1:E:138:SER:O	1:E:140:ASP:N	2.49	0.46
1:E:279:VAL:HG11	1:G:204:VAL:CG2	2.34	0.46
1:E:5:ILE:HG22	1:E:29:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:VAL:O	1:G:130:VAL:C	2.54	0.46
1:H:32:ASP:O	1:H:75:SER:HB2	2.15	0.46
2:N:58:ASP:N	2:N:59:PRO:CD	2.78	0.46
1:Q:43:LEU:HA	1:Q:43:LEU:HD23	1.71	0.46
1:A:171:THR:HG23	1:C:306:LYS:HZ3	1.81	0.46
1:A:2:LYS:HB3	1:A:28:ILE:HD11	1.98	0.46
1:A:277:PRO:O	1:C:194:ARG:HG2	2.15	0.46
1:D:146:ASN:ND2	1:D:321:VAL:CG2	2.78	0.46
1:E:85:LYS:HB2	1:E:112:GLY:CA	2.44	0.46
1:G:162:ASP:C	1:G:164:LYS:H	2.19	0.46
1:H:142:PRO:HG2	1:H:143:ILE:H	1.81	0.46
1:H:232:VAL:O	1:H:234:THR:N	2.41	0.46
1:H:81:LEU:H	1:H:81:LEU:HD12	1.80	0.46
2:I:71:ASN:HA	2:I:74:ARG:CZ	2.44	0.46
1:G:181:ASP:CG	2:M:76:TYR:H	2.18	0.46
1:O:126:PRO:CG	1:O:141:GLU:HG2	2.44	0.46
1:C:187:ALA:O	1:C:196:ALA:HB1	2.16	0.46
1:C:18(B):HIS:C	1:C:20:ARG:H	2.19	0.46
1:C:4:ALA:HB2	1:C:89:ILE:HG12	1.98	0.46
1:D:102:ARG:O	1:D:106:GLY:N	2.41	0.46
1:D:139:HIS:HE1	1:D:332:TRP:CD2	2.34	0.46
1:D:162:ASP:HA	1:D:167:ILE:H	1.81	0.46
1:E:114:LYS:HB2	1:E:332:TRP:HH2	1.81	0.46
1:F:109:ILE:N	1:F:109:ILE:HD12	2.30	0.46
1:H:76:ASN:HB3	1:H:82:LEU:HD23	1.98	0.46
1:H:79:PRO:CG	1:H:99:PHE:HZ	2.26	0.46
2:I:67:ASN:HB3	2:I:70:THR:HG23	1.98	0.46
2:M:71:ASN:OD1	2:M:74:ARG:NH2	2.46	0.46
1:O:171:THR:O	1:O:242:LEU:HD12	2.16	0.46
1:Q:26:ASP:OD1	1:Q:69:LYS:HE2	2.16	0.46
1:A:301:GLY:O	1:A:302:ASP:HB2	2.16	0.46
1:C:271:LEU:HD12	1:C:290:THR:O	2.16	0.46
1:D:133:ASN:ND2	1:D:217:VAL:CA	2.79	0.46
1:D:181:ASP:OD1	1:D:195:ARG:HD3	2.16	0.46
1:D:210:ALA:O	1:D:214:VAL:HG23	2.15	0.46
1:E:221:LEU:HD22	1:E:221:LEU:N	2.30	0.46
1:H:23:SER:C	1:H:25:LEU:H	2.19	0.46
1:H:260:ARG:HG3	1:H:260:ARG:HH11	1.80	0.46
1:H:94:GLU:OE1	1:H:99:PHE:HD2	1.97	0.46
1:O:129:VAL:N	1:O:133:ASN:HD21	2.08	0.46
1:O:179:THR:C	1:O:181:ASP:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:OG1	1:A:251:PHE:N	2.49	0.46
1:B:260:ARG:O	1:B:263:ALA:HB3	2.16	0.46
1:B:281:VAL:CB	1:D:202:ASN:HD21	2.28	0.46
1:C:322:VAL:O	1:C:325:ALA:HB3	2.15	0.46
1:C:333:LYS:HB2	1:C:333:LYS:HZ2	1.80	0.46
1:D:195:ARG:NE	5:D:502:HOH:O	2.48	0.46
1:D:139:HIS:HD2	1:D:333:LYS:HD2	1.81	0.46
1:E:129:VAL:H	1:E:133:ASN:HD21	1.62	0.46
1:E:183:ARG:HG2	1:E:196:ALA:HA	1.97	0.46
1:F:133:ASN:HD22	1:F:133:ASN:H	1.64	0.46
1:F:220:ASN:C	1:F:221:LEU:HD22	2.36	0.46
1:F:64:ILE:HD13	1:F:66:VAL:HG23	1.99	0.46
1:G:211:ALA:CB	1:G:226:ASN:HA	2.38	0.46
1:G:273:VAL:HG13	1:G:292:ILE:O	2.16	0.46
1:H:101:ASP:OD1	1:H:103:GLU:HB3	2.16	0.46
1:H:183:ARG:HG3	1:H:187:ALA:HB3	1.98	0.46
1:H:301:GLY:O	1:H:302:ASP:HB2	2.16	0.46
1:H:55:ALA:O	1:H:56:ASP:CB	2.63	0.46
2:N:70:THR:HG22	2:N:72:GLU:OE2	2.16	0.46
1:B:149:CYS:HB3	3:B:401:NAD:H4N	1.97	0.45
1:C:281:VAL:O	1:C:283:PHE:N	2.49	0.45
1:D:285:CYS:HA	1:D:315:TRP:CD1	2.51	0.45
1:E:119:THR:HG22	1:E:321:VAL:CG1	2.42	0.45
1:E:200:ALA:O	1:E:233:PRO:HB3	2.15	0.45
1:H:85:LYS:CB	1:H:112:GLY:HA3	2.45	0.45
2:L:72:GLU:HB3	1:Q:188:SER:O	2.16	0.45
1:A:146:ASN:HD22	1:A:321:VAL:HG22	1.80	0.45
1:D:94:GLU:OE1	1:D:99:PHE:HD2	1.99	0.45
1:E:168:ILE:HD12	1:E:245:GLN:HG2	1.98	0.45
1:E:270:ILE:O	1:E:270:ILE:CG2	2.65	0.45
1:F:221:LEU:HD22	1:F:221:LEU:N	2.31	0.45
1:G:243:VAL:CG2	1:G:306:LYS:HE2	2.46	0.45
1:A:139:HIS:CD2	1:A:333:LYS:HB3	2.51	0.45
1:A:206:THR:HG23	1:A:229:ALA:HB3	1.97	0.45
1:A:133:ASN:OD1	1:A:217:VAL:HG12	2.17	0.45
1:C:91:ILE:HD11	1:C:93:ILE:HD12	1.98	0.45
1:D:28:ILE:HD13	1:D:28:ILE:H	1.80	0.45
1:E:109:ILE:HG13	1:E:110:GLU:N	2.31	0.45
1:E:177:SER:OG	1:E:237:VAL:O	2.32	0.45
1:E:257:ALA:HA	1:E:260:ARG:HH11	1.82	0.45
1:E:37:VAL:HG23	1:E:38:LYS:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:MET:CB	1:H:226:ASN:HD21	2.29	0.45
1:H:211:ALA:CB	1:H:226:ASN:HA	2.46	0.45
1:O:17:ARG:HD2	1:O:53:PHE:CD1	2.51	0.45
1:Q:175:THR:HB	1:Q:239:VAL:HG12	1.98	0.45
1:B:184:LEU:O	1:B:185:LEU:HD23	2.16	0.45
1:B:232:VAL:O	1:B:234:THR:N	2.40	0.45
1:E:96:THR:HB	1:E:98:VAL:HG22	1.98	0.45
1:F:0:LYS:HD2	1:F:24:PRO:CA	2.46	0.45
1:F:133:ASN:CG	1:F:217:VAL:HG12	2.36	0.45
1:F:206:THR:HG22	1:F:229:ALA:HB3	1.97	0.45
1:H:125:ILE:HD12	1:H:143:ILE:HG22	1.98	0.45
1:F:169:LYS:NZ	1:H:303:ASP:OD1	2.49	0.45
2:I:63:TYR:CE2	2:I:70:THR:HG21	2.52	0.45
1:O:115:LYS:NZ	1:O:137:TYR:OH	2.37	0.45
1:O:255:VAL:O	1:O:258:ALA:HB3	2.16	0.45
1:Q:93:ILE:HG22	1:Q:93:ILE:O	2.16	0.45
1:A:29:ALA:O	1:A:30:ILE:HD13	2.17	0.45
1:B:162:ASP:HA	1:B:167:ILE:H	1.81	0.45
1:B:183:ARG:HG2	1:B:196:ALA:HA	1.99	0.45
1:B:294:SER:C	1:B:296:LEU:H	2.20	0.45
1:D:133:ASN:O	1:D:133:ASN:OD1	2.34	0.45
1:D:21:LYS:H	1:D:21:LYS:HG2	1.60	0.45
1:D:323:ASP:O	1:D:325:ALA:N	2.49	0.45
1:F:285:CYS:O	1:F:315:TRP:CD1	2.69	0.45
1:G:152:ASN:O	1:G:156:PRO:HG2	2.17	0.45
1:H:211:ALA:HB1	1:H:226:ASN:HA	1.98	0.45
2:I:74:ARG:HB2	2:I:74:ARG:HH21	1.80	0.45
2:L:57:SER:HB2	2:L:59:PRO:HD3	1.98	0.45
1:A:215:ALA:HB2	1:A:222:LYS:HA	1.98	0.45
1:B:28:ILE:HD11	1:B:89:ILE:CD1	2.47	0.45
1:D:172:MET:HG2	1:D:173:THR:N	2.31	0.45
1:D:32:ASP:OD1	3:D:401:NAD:H1B	2.16	0.45
1:D:38:LYS:C	1:D:40:ALA:H	2.19	0.45
1:E:10:ARG:HH21	1:E:314:GLU:CD	2.20	0.45
1:F:260:ARG:O	1:F:264:GLU:OE2	2.35	0.45
1:G:173:THR:OG1	1:G:228:ILE:HD11	2.17	0.45
1:G:187:ALA:O	1:G:196:ALA:HB1	2.17	0.45
1:H:32:ASP:HA	3:H:401:NAD:N3A	2.32	0.45
1:D:62:THR:HG22	1:H:62:THR:CG2	2.47	0.45
1:D:62:THR:HB	1:H:74:VAL:HG22	1.97	0.45
2:J:73:CYS:O	2:J:74:ARG:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:69:GLU:CD	1:O:77:ARG:NH2	2.68	0.45
1:B:281:VAL:HG12	1:D:202:ASN:ND2	2.28	0.45
1:C:91:ILE:HA	1:C:115:LYS:O	2.17	0.45
1:D:162:ASP:HB2	1:D:167:ILE:HD12	1.99	0.45
1:D:165:PHE:HA	1:D:248:LYS:HB3	1.98	0.45
1:D:260:ARG:NH2	4:D:402:SO4:O3	2.48	0.45
1:E:-1:ALA:CB	1:E:26:ASP:HB2	2.46	0.45
1:F:119:THR:O	1:F:120:ALA:HB2	2.17	0.45
1:F:144:ILE:C	1:F:144:ILE:CD1	2.85	0.45
1:F:272:ASP:OD1	1:F:273:VAL:N	2.49	0.45
1:H:163:GLN:CB	1:H:164:LYS:HD2	2.47	0.45
1:H:79:PRO:O	1:H:80:SER:C	2.55	0.45
2:L:59:PRO:C	2:L:61:GLU:H	2.20	0.45
1:A:37:VAL:HG21	1:A:63:ALA:N	2.24	0.45
1:B:152:ASN:HD22	1:B:320:ARG:HG3	1.81	0.45
1:D:218:LEU:HB3	1:D:221:LEU:HD23	1.97	0.45
1:E:114:LYS:HB2	1:E:332:TRP:CH2	2.52	0.45
1:E:90:ASP:O	1:E:114:LYS:HB2	2.16	0.45
1:H:330:ASN:N	1:H:330:ASN:HD22	2.15	0.45
1:B:162:ASP:HA	1:B:167:ILE:HG13	1.99	0.45
1:D:195:ARG:NH1	2:I:75:THR:HG23	2.32	0.45
1:D:54:ASP:O	1:D:55:ALA:CB	2.63	0.45
1:E:151:THR:HG23	1:E:214:VAL:CG2	2.47	0.45
1:E:217:VAL:O	1:E:218:LEU:HD23	2.16	0.45
1:E:178:TYR:CE1	1:E:235:PRO:HA	2.52	0.45
1:E:267:LEU:CD1	1:E:271:LEU:HD13	2.44	0.45
1:E:28:ILE:HA	1:E:71:ILE:CD1	2.40	0.45
1:F:10:ARG:NH1	1:G:186:ASP:HB2	2.32	0.45
1:F:98:VAL:HG23	1:F:99:PHE:CD2	2.52	0.45
1:G:162:ASP:O	1:G:164:LYS:N	2.49	0.45
1:G:16:LEU:C	1:G:16:LEU:HD23	2.37	0.45
1:H:163:GLN:HB3	1:H:164:LYS:HD2	1.99	0.45
1:H:307:VAL:C	1:H:308:ILE:HD13	2.37	0.45
1:H:79:PRO:HG2	1:H:99:PHE:CE1	2.52	0.45
2:K:74:ARG:HA	5:K:115:HOH:O	2.16	0.45
2:K:76:TYR:CD2	2:K:76:TYR:N	2.83	0.45
2:K:78:ASN:HB3	1:O:150:THR:OG1	2.17	0.45
1:O:98:VAL:HG23	1:O:99:PHE:CD2	2.52	0.45
1:Q:32:ASP:O	1:Q:34:GLY:N	2.50	0.45
1:A:281:VAL:HG11	1:B:48:SER:HA	1.99	0.45
1:B:20:ARG:NH1	1:B:20:ARG:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:VAL:HG23	1:B:311:TYR:CE1	2.52	0.45
1:E:108:HIS:HB2	1:E:116:VAL:HG21	1.97	0.45
1:E:153:CYS:O	1:E:156:PRO:HD2	2.17	0.45
1:E:46:TYR:HD1	1:E:52:ILE:HG22	1.82	0.45
1:F:294:SER:C	1:F:296:LEU:H	2.20	0.45
1:G:262:SER:C	1:G:267:LEU:HB2	2.37	0.45
2:L:55:ASP:OD2	2:L:55:ASP:N	2.49	0.45
1:O:194:ARG:CZ	1:Q:277:PRO:HA	2.47	0.45
1:O:224:LYS:O	1:O:225:LEU:HD23	2.17	0.45
1:D:141:GLU:OE1	1:D:141:GLU:HA	2.17	0.44
1:D:169:LYS:HZ1	1:D:245:GLN:HE22	1.64	0.44
1:F:138:SER:O	1:F:141:GLU:OE1	2.35	0.44
1:G:179:THR:O	1:G:181:ASP:N	2.50	0.44
1:H:179:THR:O	1:H:181:ASP:N	2.50	0.44
1:F:277:PRO:HG2	1:H:193:LEU:HD12	1.99	0.44
1:H:168:ILE:HG21	1:H:245:GLN:OE1	2.17	0.44
1:Q:155:ALA:HB3	1:Q:156:PRO:HD3	1.99	0.44
1:B:197:ARG:NH1	1:B:197:ARG:HG3	2.32	0.44
1:B:30:ILE:HG22	1:B:31:ASN:N	2.31	0.44
1:C:18(A):TRP:CE2	1:C:27:ILE:HD13	2.51	0.44
1:C:191:ARG:HG3	1:C:192:ASP:N	2.31	0.44
1:D:106:GLY:O	1:D:108:HIS:N	2.50	0.44
1:F:161:LEU:O	1:F:165:PHE:HB2	2.17	0.44
1:G:167:ILE:HD12	1:G:244:VAL:HG21	1.99	0.44
1:O:251:PHE:CE2	1:O:253:GLU:HB2	2.51	0.44
1:A:193:LEU:HG	5:A:509:HOH:O	2.18	0.44
1:A:37:VAL:HG13	1:A:64:ILE:CG2	2.46	0.44
1:D:151:THR:OG1	1:D:210:ALA:HA	2.18	0.44
1:E:118:ILE:HD12	1:E:118:ILE:N	2.32	0.44
1:E:5:ILE:HD13	1:E:6:ASN:N	2.33	0.44
1:F:132:VAL:HG11	1:F:218:LEU:HG	1.99	0.44
1:F:16:LEU:CD2	1:F:44:LEU:HD21	2.48	0.44
1:G:221:LEU:O	1:G:221:LEU:HG	2.17	0.44
1:O:70:ILE:HD12	1:O:70:ILE:N	2.33	0.44
1:A:16:LEU:HD23	1:A:16:LEU:C	2.38	0.44
1:B:73:VAL:O	1:B:73:VAL:HG12	2.16	0.44
1:E:172:MET:HA	1:E:242:LEU:HA	1.99	0.44
1:E:243:VAL:HG21	1:G:171:THR:HG21	1.99	0.44
1:E:161:LEU:HD21	1:E:305:VAL:HG11	1.98	0.44
1:G:98:VAL:HG23	1:G:99:PHE:CD2	2.51	0.44
1:H:9:GLY:N	3:H:401:NAD:H4B	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:4:ALA:HB2	1:Q:89:ILE:CG1	2.40	0.44
1:D:109:ILE:HG13	1:D:110:GLU:N	2.32	0.44
1:D:17:ARG:NH1	1:D:53:PHE:HB2	2.33	0.44
1:D:214:VAL:HB	1:D:225:LEU:HD12	1.99	0.44
1:D:79:PRO:HG3	1:D:99:PHE:CE2	2.52	0.44
1:E:79:PRO:HB3	1:E:108:HIS:ND1	2.33	0.44
1:E:179:THR:O	1:E:181:ASP:N	2.50	0.44
1:H:167:ILE:HD12	1:H:221:LEU:HD11	1.99	0.44
1:H:224:LYS:O	1:H:225:LEU:HD23	2.18	0.44
1:H:153:CYS:HA	1:H:289:SER:O	2.17	0.44
2:L:57:SER:C	2:L:59:PRO:HD3	2.37	0.44
1:Q:284:ARG:O	1:Q:285:CYS:HB2	2.18	0.44
1:Q:98:VAL:HG23	1:Q:99:PHE:CD2	2.53	0.44
1:A:226:ASN:ND2	1:C:300:MET:HB2	2.32	0.44
1:D:215:ALA:HB1	1:D:222:LYS:HD2	2.00	0.44
1:D:71:ILE:O	1:D:72:GLN:C	2.56	0.44
1:E:115:LYS:HD3	1:E:328:VAL:CG1	2.48	0.44
1:E:125:ILE:HG23	1:E:143:ILE:O	2.16	0.44
1:H:44:LEU:HB3	1:H:57:VAL:HG11	1.98	0.44
1:B:52:ILE:CD1	1:B:52:ILE:N	2.80	0.44
1:C:167:ILE:HG23	1:C:244:VAL:HB	2.00	0.44
1:C:174:THR:HA	1:C:240:VAL:HA	2.00	0.44
1:C:281:VAL:O	1:C:284:ARG:HG2	2.16	0.44
1:D:201:LEU:HD23	1:D:201:LEU:N	2.33	0.44
1:D:204:VAL:HB	1:D:231:ARG:HB2	1.99	0.44
1:E:39:GLN:NE2	1:E:39:GLN:N	2.65	0.44
1:F:178:TYR:CD1	1:F:178:TYR:C	2.91	0.44
1:G:101:ASP:O	1:G:104:GLY:N	2.50	0.44
1:H:135:ASP:C	1:H:137:TYR:H	2.20	0.44
1:H:99:PHE:HB3	1:H:105:ALA:HB2	1.98	0.44
2:N:68:PRO:O	2:N:73:CYS:HB2	2.16	0.44
2:K:74:ARG:O	1:O:181:ASP:OD1	2.35	0.44
1:O:86:GLU:H	1:O:86:GLU:CD	2.18	0.44
1:A:28:ILE:C	1:A:71:ILE:HG13	2.38	0.44
1:B:114:LYS:HB2	1:B:114:LYS:HZ2	1.83	0.44
1:C:87:LEU:HD12	1:C:89:ILE:HD11	2.00	0.44
1:D:293:ASP:HB3	1:D:296:LEU:HD12	2.00	0.44
1:D:249:LYS:CD	1:D:302:ASP:HB3	2.41	0.44
1:D:39:GLN:O	1:D:43:LEU:HD12	2.18	0.44
1:D:75:SER:HB3	1:H:61:GLU:HB2	2.00	0.44
1:E:194:ARG:HE	1:G:277:PRO:C	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:VAL:CG2	1:E:240:VAL:N	2.80	0.44
1:E:280:SER:HB3	1:G:202:ASN:CB	2.48	0.44
1:F:27:ILE:C	1:F:28:ILE:HD12	2.38	0.44
1:Q:287:ASP:OD1	1:Q:315:TRP:NE1	2.42	0.44
1:A:172:MET:HE1	1:A:210:ALA:HB3	2.00	0.44
1:A:300:MET:HG3	1:C:169:LYS:HB2	1.99	0.44
1:B:220:ASN:C	1:B:222:LYS:H	2.20	0.44
1:B:50:LEU:HA	1:B:284:ARG:NH2	2.33	0.44
1:C:16:LEU:HD23	1:C:18(A):TRP:HE3	1.81	0.44
1:D:191:ARG:HA	2:I:60:LEU:HD23	1.99	0.44
1:D:250:THR:O	1:D:302:ASP:O	2.35	0.44
1:E:132:VAL:HG11	1:E:217:VAL:CB	2.48	0.44
1:E:194:ARG:HH12	1:G:296:LEU:HD21	1.83	0.44
1:E:129:VAL:HG21	1:E:217:VAL:HG11	2.00	0.44
1:E:58:LYS:HB3	1:E:58:LYS:HZ3	1.83	0.44
1:F:62:THR:O	1:F:63:ALA:HB2	2.17	0.44
1:E:300:MET:O	1:G:169:LYS:HE2	2.17	0.44
2:L:59:PRO:C	2:L:61:GLU:N	2.71	0.44
1:O:89:ILE:O	1:O:113:ALA:HA	2.18	0.44
1:B:91:ILE:HD11	1:B:117:ILE:HG21	2.00	0.43
1:B:129:VAL:H	1:B:133:ASN:HD21	1.66	0.43
1:C:206:THR:HG22	1:C:229:ALA:HB3	2.01	0.43
1:E:214:VAL:HG12	1:E:214:VAL:O	2.17	0.43
1:H:211:ALA:HB1	1:H:226:ASN:CA	2.48	0.43
1:H:191:ARG:CD	2:N:73:CYS:HA	2.48	0.43
1:C:21:LYS:O	1:C:21:LYS:HG2	2.18	0.43
1:F:1:LEU:HD22	1:F:329:ALA:HB1	2.00	0.43
1:F:167:ILE:HG21	1:F:221:LEU:HD11	2.00	0.43
1:G:162:ASP:HB2	1:G:167:ILE:HG12	2.00	0.43
1:G:173:THR:HG23	1:G:228:ILE:HD12	2.00	0.43
1:G:280:SER:O	1:G:282:ASP:N	2.51	0.43
1:A:109:ILE:CD1	1:A:116:VAL:HG23	2.48	0.43
1:A:200:ALA:O	1:A:201:LEU:HG	2.18	0.43
1:C:228:ILE:HD13	1:C:228:ILE:N	2.33	0.43
1:D:116:VAL:HG12	1:D:117:ILE:H	1.82	0.43
1:E:183:ARG:HH22	2:N:74:ARG:NH1	2.15	0.43
1:E:18:CYS:SG	1:E:319:GLN:OE1	2.76	0.43
1:F:105:ALA:HB1	1:F:143:ILE:HD12	2.00	0.43
1:G:262:SER:HA	1:G:266:GLU:OE2	2.18	0.43
1:E:204:VAL:HG22	1:G:279:VAL:CG1	2.49	0.43
1:G:37:VAL:HG13	1:G:73:VAL:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:ARG:HG2	1:H:53:PHE:HE1	1.81	0.43
1:Q:1:LEU:HD12	1:Q:1:LEU:HA	1.87	0.43
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.83	0.43
1:D:211:ALA:CB	1:D:226:ASN:HA	2.48	0.43
1:D:307:VAL:C	1:D:308:ILE:HD12	2.38	0.43
1:F:1:LEU:N	1:F:1:LEU:CD1	2.81	0.43
1:G:154:LEU:HD21	1:G:172:MET:HG3	1.99	0.43
1:G:158:VAL:HG11	1:G:221:LEU:HD22	1.98	0.43
1:G:176:HIS:HA	1:G:238:SER:OG	2.18	0.43
1:G:267:LEU:HD23	1:G:267:LEU:HA	1.82	0.43
1:F:193:LEU:HD21	1:G:39:GLN:HG2	2.00	0.43
1:G:57:VAL:HA	1:G:65:SER:O	2.18	0.43
1:H:204:VAL:HB	1:H:231:ARG:HB2	2.00	0.43
1:H:3:VAL:HG22	1:H:4:ALA:N	2.33	0.43
1:H:79:PRO:HG3	1:H:99:PHE:HZ	1.83	0.43
1:A:109:ILE:C	1:A:111:ALA:N	2.72	0.43
1:A:125:ILE:CG2	1:A:143:ILE:HG22	2.47	0.43
1:A:149:CYS:HB3	3:A:401:NAD:H4N	2.00	0.43
1:B:195:ARG:NH1	2:J:76:TYR:H	2.16	0.43
1:B:194:ARG:HD2	1:B:205:PRO:HD2	2.00	0.43
1:B:84:TRP:CE3	1:B:84:TRP:HA	2.53	0.43
1:C:177:SER:OG	1:C:237:VAL:O	2.28	0.43
1:D:23:SER:OG	1:D:24:PRO:HD2	2.18	0.43
1:E:153:CYS:O	1:E:290:THR:CG2	2.66	0.43
1:E:20:ARG:HH12	1:E:322:VAL:HG12	1.82	0.43
1:E:161:LEU:HD13	1:E:244:VAL:CG2	2.49	0.43
1:F:91:ILE:HD11	1:F:117:ILE:HD12	2.00	0.43
1:F:128:TYR:HA	1:F:133:ASN:ND2	2.34	0.43
1:F:206:THR:CG2	1:F:229:ALA:HB3	2.48	0.43
2:I:76:TYR:CD1	2:I:76:TYR:N	2.85	0.43
1:Q:110:GLU:C	1:Q:112:GLY:N	2.71	0.43
1:Q:159:LYS:O	1:Q:163:GLN:HG3	2.17	0.43
1:Q:191:ARG:HG3	1:Q:191:ARG:NH1	2.32	0.43
1:Q:211:ALA:HB1	1:Q:226:ASN:HA	2.01	0.43
1:A:184:LEU:HG	1:A:185:LEU:CD1	2.43	0.43
1:B:8:PHE:CE1	1:B:16:LEU:HD12	2.53	0.43
1:D:191:ARG:HH22	2:I:61:GLU:HB3	1.82	0.43
1:F:107:LYS:HA	1:F:110:GLU:CG	2.49	0.43
1:F:232:VAL:HG11	1:H:232:VAL:HG11	2.00	0.43
1:H:17:ARG:HD3	1:H:50:LEU:CD1	2.49	0.43
1:F:226:ASN:HB3	1:H:300:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:ILE:HD12	1:O:27:ILE:N	2.33	0.43
1:A:124:ASP:HB3	4:A:406:SO4:O2	2.18	0.43
1:B:198:ALA:CB	1:B:201:LEU:HD12	2.48	0.43
1:B:31:ASN:HB2	1:B:74:VAL:HG22	2.00	0.43
1:B:50:LEU:HD23	1:B:284:ARG:HH22	1.83	0.43
1:A:281:VAL:HG12	1:C:202:ASN:HD21	1.83	0.43
1:E:167:ILE:HG23	1:E:244:VAL:HB	2.00	0.43
1:E:239:VAL:HG23	1:E:309:ALA:O	2.18	0.43
1:E:30:ILE:HG13	1:E:71:ILE:CG2	2.48	0.43
1:E:39:GLN:H	1:E:39:GLN:NE2	2.16	0.43
1:E:4:ALA:HB3	1:E:92:VAL:HG22	1.99	0.43
1:E:96:THR:CB	1:E:98:VAL:HG22	2.49	0.43
1:H:29:ALA:C	1:H:30:ILE:HG13	2.38	0.43
1:H:328:VAL:O	1:H:332:TRP:HB2	2.19	0.43
1:H:69:LYS:HE2	1:H:70:ILE:HD13	1.99	0.43
2:M:70:THR:HG22	2:M:71:ASN:H	1.82	0.43
1:D:153:CYS:HA	1:D:289:SER:O	2.18	0.43
1:D:266:GLU:HG2	1:D:267:LEU:HG	2.01	0.43
1:E:169:LYS:HB2	1:E:169:LYS:HE2	1.73	0.43
1:E:37:VAL:O	1:E:41:SER:CB	2.67	0.43
1:F:152:ASN:ND2	1:F:317:TYR:CE1	2.87	0.43
1:F:159:LYS:O	1:F:163:GLN:HG3	2.19	0.43
1:F:190:HIS:CB	1:F:196:ALA:HB2	2.44	0.43
1:F:78:ASN:OD1	1:F:80:SER:HB2	2.19	0.43
1:G:132:VAL:C	1:G:134:ALA:H	2.22	0.43
1:G:160:VAL:O	1:G:164:LYS:HB3	2.19	0.43
1:E:300:MET:CB	1:G:169:LYS:HD3	2.49	0.43
1:G:182:GLN:HB3	1:G:199:ALA:HB2	2.01	0.43
1:G:214:VAL:CG1	1:G:218:LEU:HD12	2.49	0.43
1:G:146:ASN:OD1	1:G:324:LEU:HD22	2.19	0.43
1:E:193:LEU:HD22	1:H:42:HIS:HB3	2.00	0.43
1:H:8:PHE:CE2	1:H:13:ARG:HG2	2.53	0.43
1:O:15:PHE:O	1:O:18:CYS:HB2	2.19	0.43
1:Q:139:HIS:C	1:Q:141:GLU:H	2.20	0.43
1:A:129:VAL:N	1:A:133:ASN:HD21	2.12	0.43
1:A:82:LEU:C	1:A:84:TRP:H	2.22	0.43
1:B:284:ARG:HG2	1:B:284:ARG:HH11	1.83	0.43
1:C:239:VAL:CG2	1:C:308:ILE:HG23	2.49	0.43
1:C:54:ASP:O	1:C:55:ALA:HB2	2.19	0.43
1:D:206:THR:HG21	1:D:231:ARG:NH1	2.34	0.43
1:D:240:VAL:HG13	1:D:311:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:SER:O	1:D:267:LEU:HB2	2.19	0.43
1:E:242:LEU:CD1	1:E:244:VAL:HG13	2.45	0.43
1:E:15:PHE:CE2	1:E:93:ILE:HD13	2.54	0.43
1:F:228:ILE:HG12	1:F:229:ALA:N	2.33	0.43
1:G:174:THR:HG22	1:G:229:ALA:HA	2.01	0.43
1:G:327:ILE:CD1	1:G:327:ILE:N	2.82	0.43
1:H:161:LEU:O	1:H:165:PHE:HB2	2.19	0.43
1:H:29:ALA:HA	1:H:71:ILE:CG2	2.49	0.43
1:O:253:GLU:CD	1:O:253:GLU:N	2.72	0.43
1:A:0:LYS:H1	1:A:0:LYS:HG3	1.67	0.43
1:A:188:SER:HB2	1:D:39:GLN:NE2	2.33	0.43
1:B:202:ASN:O	1:B:233:PRO:HD3	2.19	0.43
1:A:306:LYS:HD2	1:C:171:THR:OG1	2.18	0.43
1:C:317:TYR:O	1:C:320:ARG:HB2	2.19	0.43
1:E:293:ASP:OD1	1:E:296:LEU:HG	2.19	0.43
1:E:45:LYS:O	1:E:52:ILE:HA	2.19	0.43
1:G:162:ASP:CB	1:G:167:ILE:HG12	2.49	0.43
1:G:319:GLN:OE1	1:G:319:GLN:HA	2.18	0.43
1:H:190:HIS:HA	2:N:72:GLU:O	2.19	0.43
1:Q:125:ILE:HA	1:Q:126:PRO:HD3	1.97	0.43
1:Q:261:ASP:O	1:Q:265:LYS:HG3	2.19	0.43
1:A:139:HIS:CE1	1:A:332:TRP:HA	2.54	0.42
1:A:173:THR:HG23	1:A:228:ILE:HD12	2.01	0.42
1:C:1:LEU:CD2	1:C:329:ALA:HA	2.48	0.42
1:E:299:VAL:HG13	1:E:304:MET:C	2.39	0.42
1:F:133:ASN:ND2	1:F:133:ASN:N	2.66	0.42
1:F:152:ASN:HD21	1:F:317:TYR:HE1	1.67	0.42
1:F:250:THR:OG1	1:F:251:PHE:N	2.51	0.42
1:G:125:ILE:HA	1:G:126:PRO:HD3	1.88	0.42
1:H:39:GLN:O	1:H:43:LEU:HG	2.18	0.42
1:B:197:ARG:HH11	1:B:197:ARG:HG3	1.83	0.42
1:B:129:VAL:HG23	1:B:217:VAL:HG11	2.00	0.42
1:B:262:SER:O	1:B:265:LYS:N	2.50	0.42
1:C:263:ALA:O	1:C:268:LYS:HA	2.18	0.42
1:C:281:VAL:C	1:C:283:PHE:N	2.73	0.42
1:E:239:VAL:CG2	1:E:240:VAL:H	2.28	0.42
1:H:82:LEU:HD13	1:H:84:TRP:CZ2	2.53	0.42
2:M:60:LEU:O	2:M:63:TYR:N	2.52	0.42
1:A:139:HIS:CB	1:A:333:LYS:HE2	2.48	0.42
1:C:132:VAL:HG21	1:C:155:ALA:HB1	2.01	0.42
1:A:193:LEU:HD12	1:C:277:PRO:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH2	1:C:282:ASP:OD1	2.44	0.42
1:C:313:ASN:HB2	3:C:401:NAD:O7N	2.18	0.42
1:D:119:THR:O	1:D:120:ALA:HB2	2.19	0.42
1:D:191:ARG:HH12	2:I:61:GLU:HG2	1.83	0.42
1:E:208:THR:HB	1:E:229:ALA:HB2	2.02	0.42
1:F:239:VAL:HG13	1:F:239:VAL:O	2.18	0.42
1:F:173:THR:O	1:F:241:ASP:HB3	2.19	0.42
1:F:60:SER:O	1:F:63:ALA:HB3	2.19	0.42
1:H:3:VAL:O	1:H:28:ILE:HG22	2.18	0.42
1:O:125:ILE:HA	1:O:126:PRO:HD3	1.93	0.42
1:O:251:PHE:O	1:O:254:GLU:HB3	2.19	0.42
1:O:298:MET:CE	1:Q:226:ASN:ND2	2.82	0.42
1:A:9:GLY:O	1:A:13:ARG:HG3	2.20	0.42
1:A:226:ASN:C	1:A:226:ASN:OD1	2.58	0.42
1:A:279:VAL:HG22	1:C:197:ARG:HH12	1.84	0.42
1:B:177:SER:HB3	1:B:234:THR:O	2.20	0.42
1:C:218:LEU:HB3	1:C:221:LEU:HD23	2.02	0.42
1:C:266:GLU:HG2	1:C:267:LEU:H	1.84	0.42
1:D:144:ILE:CD1	1:D:145:SER:N	2.81	0.42
1:D:172:MET:HG2	1:D:173:THR:H	1.84	0.42
1:D:190:HIS:C	2:I:60:LEU:HD21	2.39	0.42
1:D:31:ASN:OD1	1:D:74:VAL:HG23	2.19	0.42
1:C:253:GLU:HG2	1:E:103:GLU:HG3	2.01	0.42
1:E:278:LEU:HD21	1:F:46:TYR:CE2	2.53	0.42
1:F:85:LYS:N	1:F:112:GLY:HA3	2.35	0.42
1:F:134:ALA:C	1:F:136:ALA:H	2.21	0.42
1:F:142:PRO:O	1:F:143:ILE:HD13	2.19	0.42
1:F:222:LYS:NZ	1:F:224:LYS:HE2	2.35	0.42
1:F:280:SER:OG	1:H:202:ASN:CB	2.67	0.42
1:F:34:GLY:HA2	2:M:60:LEU:HB2	2.00	0.42
1:G:154:LEU:HD12	1:G:240:VAL:HG11	2.01	0.42
1:G:252:ALA:O	1:G:255:VAL:HB	2.19	0.42
1:G:84:TRP:HA	1:G:84:TRP:HE3	1.85	0.42
1:H:10:ARG:HB2	3:H:401:NAD:O2N	2.20	0.42
1:H:114:LYS:O	1:H:115:LYS:HG3	2.20	0.42
1:F:202:ASN:ND2	1:H:281:VAL:CG2	2.74	0.42
1:H:32:ASP:O	1:H:75:SER:CB	2.68	0.42
1:B:114:LYS:NZ	1:B:114:LYS:HB2	2.35	0.42
1:C:116:VAL:HG12	1:C:117:ILE:N	2.34	0.42
1:C:9:GLY:HA3	3:C:401:NAD:O5B	2.20	0.42
1:D:181:ASP:OD1	1:D:195:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:ILE:HA	1:E:126:PRO:HD3	1.90	0.42
1:F:285:CYS:HA	1:F:315:TRP:CG	2.55	0.42
1:F:63:ALA:HB2	1:F:72:GLN:OE1	2.19	0.42
1:H:90:ASP:HA	1:H:114:LYS:HD2	2.02	0.42
1:H:250:THR:CB	1:H:254:GLU:OE1	2.68	0.42
1:H:79:PRO:O	1:H:82:LEU:HG	2.19	0.42
1:H:8:PHE:CZ	1:H:16:LEU:HD12	2.54	0.42
1:Q:164:LYS:O	1:Q:248:LYS:HD3	2.19	0.42
1:B:234:THR:CG2	1:D:233:PRO:HG2	2.49	0.42
1:C:115:LYS:NZ	1:C:115:LYS:HB2	2.35	0.42
1:B:296:LEU:CD2	1:D:228:ILE:HG21	2.44	0.42
1:D:319:GLN:NE2	1:D:319:GLN:CA	2.81	0.42
1:E:194:ARG:HE	1:G:277:PRO:CB	2.32	0.42
1:F:32:ASP:HA	3:F:401:NAD:C2A	2.50	0.42
1:G:152:ASN:O	1:G:289:SER:HB3	2.20	0.42
1:G:256:ASN:HB3	1:G:260:ARG:HH12	1.84	0.42
1:G:327:ILE:HD12	1:G:327:ILE:N	2.34	0.42
1:H:108:HIS:HB2	1:H:116:VAL:HG21	2.02	0.42
1:H:23:SER:O	1:H:25:LEU:N	2.42	0.42
1:H:280:SER:O	1:H:281:VAL:C	2.58	0.42
1:H:5:ILE:HB	1:H:30:ILE:HG23	2.02	0.42
1:A:324:LEU:O	1:A:327:ILE:HB	2.20	0.42
1:A:39:GLN:CD	1:A:39:GLN:H	2.23	0.42
1:D:155:ALA:H	1:D:156:PRO:CD	2.32	0.42
1:E:137:TYR:CZ	1:E:139:HIS:HA	2.54	0.42
1:E:179:THR:C	1:E:181:ASP:N	2.73	0.42
1:E:62:THR:O	1:E:63:ALA:HB2	2.19	0.42
1:F:31:ASN:HB2	1:F:74:VAL:HG13	2.02	0.42
1:G:171:THR:HG22	1:G:243:VAL:HB	2.00	0.42
3:H:401:NAD:O1A	2:N:76:TYR:OH	2.37	0.42
1:H:41:SER:CB	1:H:59:PRO:HG3	2.50	0.42
1:H:41:SER:HA	1:H:57:VAL:HG12	2.00	0.42
1:O:274:CYS:SG	1:O:278:LEU:HD12	2.60	0.42
1:O:298:MET:HE1	1:Q:226:ASN:CB	2.49	0.42
1:A:5:ILE:HD11	1:A:27:ILE:HD12	2.01	0.42
1:B:253:GLU:H	1:B:253:GLU:CD	2.23	0.42
1:B:84:TRP:HA	1:B:84:TRP:HE3	1.84	0.42
1:C:262:SER:C	1:C:264:GLU:H	2.22	0.42
1:D:183:ARG:HG3	1:D:187:ALA:HB3	2.01	0.42
1:D:316:GLY:O	1:D:319:GLN:HB2	2.19	0.42
1:E:285:CYS:HA	1:E:315:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:ASN:CB	1:G:260:ARG:NH1	2.83	0.42
1:H:150:THR:HG22	1:H:172:MET:HE2	2.01	0.42
1:H:213:ALA:O	1:H:216:LEU:HD13	2.19	0.42
1:H:63:ALA:CB	1:H:72:GLN:HA	2.49	0.42
1:H:3:VAL:HB	1:H:91:ILE:HG22	2.00	0.42
1:O:202:ASN:HD21	1:Q:281:VAL:CB	2.32	0.42
1:O:15:PHE:HA	1:O:318:SER:HB3	2.02	0.42
1:Q:129:VAL:N	1:Q:133:ASN:HD21	2.16	0.42
1:Q:33:THR:HG22	1:Q:77:ARG:HG2	2.01	0.42
1:A:173:THR:HG23	1:A:228:ILE:HD11	2.02	0.42
1:A:185:LEU:O	1:A:187:ALA:N	2.53	0.42
1:B:57:VAL:O	1:B:58:LYS:HB3	2.19	0.42
1:B:70:ILE:HD12	1:B:70:ILE:H	1.81	0.42
1:D:162:ASP:CA	1:D:167:ILE:HG13	2.48	0.42
1:B:202:ASN:ND2	1:D:281:VAL:HG12	2.33	0.42
1:D:78:ASN:HA	1:D:79:PRO:HD3	1.81	0.42
1:D:84:TRP:CE3	1:D:84:TRP:HA	2.55	0.42
1:F:178:TYR:CD1	1:F:178:TYR:O	2.73	0.42
1:F:301:GLY:O	1:F:302:ASP:HB2	2.18	0.42
1:F:56:ASP:HB2	1:F:67:ASP:HA	2.01	0.42
1:G:256:ASN:HB3	1:G:260:ARG:NH1	2.35	0.42
1:H:32:ASP:HA	3:H:401:NAD:C2A	2.50	0.42
1:Q:79:PRO:HB2	1:Q:107:LYS:HB2	2.01	0.42
1:A:1:LEU:HD21	1:A:332:TRP:CE3	2.55	0.42
1:B:271:LEU:HD22	1:B:290:THR:HG23	2.02	0.42
1:C:27:ILE:HG21	1:C:71:ILE:HD13	2.02	0.42
1:D:157:PHE:O	1:D:161:LEU:HG	2.20	0.42
1:D:280:SER:HB3	1:D:310:TRP:HZ3	1.84	0.42
1:E:139:HIS:HB3	5:E:531:HOH:O	2.19	0.42
1:G:18(A):TRP:HH2	1:G:69:LYS:HE2	1.84	0.42
1:F:300:MET:HE1	1:H:169:LYS:HB2	2.02	0.42
1:H:25:LEU:HD12	1:H:25:LEU:N	2.35	0.42
2:N:70:THR:HG22	2:N:72:GLU:HG2	2.02	0.42
1:Q:18(A):TRP:CD2	1:Q:27:ILE:HG12	2.55	0.42
1:A:301:GLY:O	1:A:302:ASP:CB	2.67	0.41
1:A:60:SER:O	1:A:63:ALA:HB3	2.20	0.41
1:C:218:LEU:O	1:C:221:LEU:HB2	2.20	0.41
1:C:24:PRO:HD2	1:C:25:LEU:HG	2.01	0.41
1:C:27:ILE:O	1:C:71:ILE:HG12	2.20	0.41
1:D:1:LEU:HD23	1:D:91:ILE:HD12	2.01	0.41
1:D:255:VAL:HG11	1:D:305:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:PRO:HD2	1:E:143:ILE:O	2.20	0.41
1:E:280:SER:O	1:E:282:ASP:N	2.53	0.41
1:F:227:GLY:HA2	1:H:298:MET:HE3	2.02	0.41
1:H:141:GLU:OE1	1:H:141:GLU:HA	2.20	0.41
1:H:250:THR:OG1	1:H:254:GLU:OE1	2.38	0.41
1:H:315:TRP:CD1	1:H:315:TRP:C	2.93	0.41
1:H:52:ILE:HD12	1:H:52:ILE:N	2.34	0.41
1:O:172:MET:O	1:O:227:GLY:HA2	2.20	0.41
1:O:76:ASN:HD21	1:O:81:LEU:HB2	1.85	0.41
1:Q:32:ASP:OD2	3:Q:401:NAD:H1B	2.20	0.41
1:B:163:GLN:C	1:B:163:GLN:CD	2.78	0.41
1:C:84:TRP:CE3	1:C:84:TRP:CA	3.02	0.41
1:E:101:ASP:OD2	1:E:103:GLU:HB3	2.20	0.41
1:E:236:ASN:CG	1:E:237:VAL:N	2.74	0.41
1:E:284:ARG:O	1:E:285:CYS:HB2	2.20	0.41
1:F:277:PRO:HG3	1:H:193:LEU:HD12	2.00	0.41
1:H:15:PHE:HE1	1:H:321:VAL:HG12	1.85	0.41
1:D:62:THR:HG21	1:H:74:VAL:HA	2.02	0.41
2:N:70:THR:CG2	2:N:72:GLU:HG2	2.50	0.41
1:O:157:PHE:HD2	1:O:290:THR:HG21	1.85	0.41
1:Q:154:LEU:HD12	1:Q:157:PHE:CZ	2.55	0.41
1:A:300:MET:HE3	1:C:226:ASN:HD22	1.79	0.41
1:C:253:GLU:HG3	4:C:404:SO4:O2	2.20	0.41
1:D:125:ILE:HD11	1:D:143:ILE:CG2	2.50	0.41
1:D:133:ASN:C	1:D:135:ASP:N	2.73	0.41
1:D:261:ASP:C	1:D:263:ALA:N	2.73	0.41
1:D:252:ALA:HA	1:D:299:VAL:HG23	2.01	0.41
1:E:109:ILE:N	1:E:113:ALA:HB3	2.35	0.41
1:E:146:ASN:HB3	1:E:317:TYR:OH	2.20	0.41
1:E:198:ALA:CB	1:E:201:LEU:HD11	2.50	0.41
1:F:101:ASP:O	1:F:102:ARG:C	2.59	0.41
1:F:138:SER:OG	1:F:140:ASP:OD1	2.36	0.41
1:F:164:LYS:O	1:F:165:PHE:CG	2.74	0.41
1:F:85:LYS:HB2	1:F:85:LYS:HE3	1.72	0.41
1:G:236:ASN:O	1:G:237:VAL:HB	2.20	0.41
1:H:32:ASP:O	1:H:75:SER:OG	2.38	0.41
1:H:45:LYS:HG3	1:H:45:LYS:O	2.20	0.41
1:Q:172:MET:CE	1:Q:211:ALA:HB2	2.50	0.41
1:A:5:ILE:HD11	1:A:27:ILE:CD1	2.50	0.41
1:B:139:HIS:CB	1:B:333:LYS:HG3	2.47	0.41
1:D:191:ARG:CZ	2:I:61:GLU:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ARG:O	1:D:285:CYS:HB2	2.21	0.41
1:E:15:PHE:CD1	1:E:322:VAL:HG22	2.54	0.41
1:E:204:VAL:HG22	1:G:279:VAL:HG11	2.02	0.41
1:E:76:ASN:HB3	1:E:82:LEU:CD2	2.51	0.41
1:F:165:PHE:HE1	1:F:250:THR:HB	1.84	0.41
1:F:254:GLU:O	1:F:257:ALA:HB3	2.18	0.41
1:G:84:TRP:CE3	1:G:84:TRP:HA	2.56	0.41
1:H:152:ASN:O	1:H:289:SER:HB3	2.19	0.41
1:H:17:ARG:NE	1:H:53:PHE:CD1	2.87	0.41
1:H:269:GLY:HA2	1:H:288:PHE:CE2	2.44	0.41
1:H:41:SER:HA	1:H:57:VAL:CG1	2.50	0.41
1:O:96:THR:OG1	1:O:98:VAL:HG22	2.20	0.41
1:Q:176:HIS:HA	1:Q:238:SER:OG	2.21	0.41
1:A:104:GLY:O	1:A:106:GLY:N	2.53	0.41
1:B:318:SER:O	1:B:322:VAL:HG23	2.19	0.41
1:C:266:GLU:C	1:C:268:LYS:H	2.22	0.41
1:C:47:ASP:C	1:C:49:THR:H	2.24	0.41
1:D:84:TRP:HA	1:D:84:TRP:HE3	1.84	0.41
1:F:170:GLY:HA3	1:F:244:VAL:HG12	2.03	0.41
1:F:3:VAL:CG1	1:F:4:ALA:N	2.83	0.41
1:G:109:ILE:CD1	1:G:116:VAL:HG23	2.50	0.41
1:G:214:VAL:HG12	1:G:218:LEU:HD12	2.02	0.41
1:H:108:HIS:C	1:H:110:GLU:N	2.74	0.41
1:H:57:VAL:O	1:H:57:VAL:HG12	2.20	0.41
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.55	0.41
1:Q:211:ALA:CB	1:Q:226:ASN:HA	2.50	0.41
1:B:120:ALA:O	1:B:145:SER:OG	2.35	0.41
1:B:8:PHE:CZ	1:B:16:LEU:HD12	2.56	0.41
1:D:29:ALA:HA	1:D:72:GLN:O	2.21	0.41
1:E:327:ILE:C	1:E:329:ALA:N	2.73	0.41
1:F:139:HIS:HD2	1:F:333:LYS:HD2	1.83	0.41
1:F:197:ARG:HH21	1:G:48:SER:N	2.19	0.41
1:G:313:ASN:HB2	3:G:401:NAD:O7N	2.19	0.41
1:H:173:THR:O	1:H:241:ASP:HB3	2.20	0.41
2:I:67:ASN:HB3	2:I:70:THR:CG2	2.50	0.41
1:B:195:ARG:CZ	2:J:75:THR:HG23	2.50	0.41
1:O:284:ARG:O	1:O:285:CYS:HB2	2.19	0.41
1:O:298:MET:CE	1:Q:226:ASN:HB3	2.50	0.41
1:A:68:GLY:O	1:A:69:LYS:C	2.58	0.41
1:A:31:ASN:OD1	1:A:74:VAL:HG23	2.20	0.41
1:D:252:ALA:HA	1:D:299:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:TYR:HD1	1:F:178:TYR:C	2.23	0.41
1:F:222:LYS:O	1:F:224:LYS:HG3	2.21	0.41
1:F:38:LYS:HE3	1:G:193:LEU:HD21	2.02	0.41
1:G:278:LEU:HD22	1:H:46:TYR:CD1	2.56	0.41
1:H:129:VAL:H	1:H:133:ASN:HD21	1.68	0.41
1:H:294:SER:C	1:H:296:LEU:H	2.23	0.41
1:H:293:ASP:CB	1:H:296:LEU:HD12	2.43	0.41
1:H:59:PRO:HA	1:H:64:ILE:HG22	2.03	0.41
1:H:63:ALA:HA	1:H:73:VAL:HG23	2.03	0.41
1:A:70:ILE:CG2	1:A:71:ILE:N	2.83	0.41
1:B:109:ILE:HG23	1:B:113:ALA:O	2.21	0.41
1:B:182:GLN:OE1	1:B:231:ARG:NH1	2.54	0.41
1:C:117:ILE:HD11	1:C:328:VAL:HG21	2.02	0.41
1:C:69:LYS:HE2	5:C:521:HOH:O	2.20	0.41
1:D:105:ALA:CB	1:D:118:ILE:HD11	2.50	0.41
1:E:116:VAL:HB	1:E:143:ILE:CD1	2.50	0.41
1:E:13:ARG:HG3	1:E:13:ARG:HH11	1.85	0.41
1:E:193:LEU:HD13	1:H:42:HIS:CG	2.56	0.41
1:Q:333:LYS:HA	1:Q:333:LYS:HD3	1.77	0.41
1:Q:37:VAL:CG2	1:Q:73:VAL:HB	2.50	0.41
1:B:221:LEU:H	1:B:221:LEU:CD2	2.34	0.41
1:B:252:ALA:O	1:B:254:GLU:N	2.53	0.41
1:D:151:THR:C	1:D:153:CYS:H	2.25	0.41
1:D:296:LEU:HD12	1:D:308:ILE:CG2	2.51	0.41
1:E:255:VAL:HG21	1:E:299:VAL:HG21	2.03	0.41
1:E:54:ASP:O	1:E:55:ALA:HB2	2.21	0.41
1:F:132:VAL:C	1:F:134:ALA:H	2.24	0.41
1:G:25:LEU:H	1:G:25:LEU:HG	1.62	0.41
1:G:284:ARG:O	1:G:285:CYS:HB2	2.21	0.41
1:D:62:THR:HG1	1:H:74:VAL:HG13	1.76	0.41
1:H:190:HIS:HA	2:N:72:GLU:CA	2.51	0.41
1:B:156:PRO:HB2	1:B:290:THR:HG21	2.03	0.41
1:C:320:ARG:HG2	1:C:320:ARG:NH1	2.36	0.41
1:E:119:THR:HB	1:E:317:TYR:HE2	1.86	0.41
1:E:65:SER:CB	1:E:70:ILE:HG22	2.51	0.41
1:F:133:ASN:ND2	1:F:133:ASN:H	2.19	0.41
1:F:210:ALA:CA	1:F:213:ALA:HB3	2.48	0.41
1:F:64:ILE:HD12	1:F:64:ILE:C	2.40	0.41
1:G:168:ILE:O	1:G:224:LYS:HD3	2.21	0.41
1:D:191:ARG:NH2	2:I:61:GLU:HG2	2.36	0.41
1:Q:85:LYS:HB2	1:Q:112:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:234:THR:HG21	1:Q:203:ILE:HG13	2.02	0.41
1:Q:82:LEU:HD13	1:Q:84:TRP:CZ2	2.55	0.41
1:A:101:ASP:OD2	1:A:103:GLU:HB3	2.20	0.41
1:A:125:ILE:HG22	1:A:144:ILE:HA	2.01	0.41
1:B:162:ASP:CA	1:B:167:ILE:HG13	2.51	0.41
1:C:262:SER:C	1:C:264:GLU:N	2.74	0.41
1:D:121:PRO:HG3	1:D:148:SER:HB3	2.02	0.41
1:A:43:LEU:HD11	1:D:187:ALA:O	2.21	0.41
1:E:6:ASN:ND2	1:E:108:HIS:CE1	2.89	0.41
1:E:66:VAL:C	1:E:68:GLY:H	2.25	0.41
1:F:37:VAL:HA	1:F:73:VAL:HG11	2.03	0.41
1:H:157:PHE:HE1	1:H:242:LEU:HD23	1.85	0.41
1:H:229:ALA:O	1:H:230:LEU:HD23	2.20	0.41
1:H:3:VAL:CG2	1:H:4:ALA:N	2.84	0.41
1:H:50:LEU:HD21	5:H:503:HOH:O	2.20	0.41
1:O:236:ASN:O	1:O:237:VAL:HB	2.20	0.41
1:O:154:LEU:CD2	1:O:240:VAL:HG11	2.45	0.41
1:Q:79:PRO:HB2	1:Q:107:LYS:CB	2.51	0.41
1:A:37:VAL:HG23	1:A:62:THR:HA	2.02	0.40
1:B:92:VAL:O	1:B:117:ILE:HG22	2.21	0.40
1:A:281:VAL:CG1	1:C:202:ASN:HD21	2.33	0.40
1:C:27:ILE:O	1:C:27:ILE:HG22	2.21	0.40
1:C:84:TRP:HB3	1:C:113:ALA:N	2.36	0.40
1:D:174:THR:O	1:D:174:THR:HG23	2.22	0.40
1:D:210:ALA:CA	1:D:213:ALA:HB3	2.51	0.40
1:D:27:ILE:C	1:D:27:ILE:HD13	2.41	0.40
1:D:28:ILE:N	1:D:28:ILE:HD13	2.37	0.40
1:E:161:LEU:O	1:E:162:ASP:C	2.60	0.40
1:E:317:TYR:O	1:E:321:VAL:HG23	2.21	0.40
1:F:228:ILE:H	1:F:228:ILE:CD1	2.34	0.40
1:F:23:SER:C	1:F:25:LEU:N	2.72	0.40
1:G:138:SER:OG	1:G:140:ASP:OD2	2.39	0.40
1:G:158:VAL:CG1	1:G:221:LEU:HD22	2.51	0.40
1:Q:179:THR:C	1:Q:181:ASP:H	2.25	0.40
1:Q:205:PRO:HA	1:Q:229:ALA:O	2.21	0.40
1:Q:84:TRP:CE3	1:Q:84:TRP:HA	2.56	0.40
1:B:25:LEU:HD11	1:B:325:ALA:HB3	2.03	0.40
1:B:32:ASP:OD2	1:B:32:ASP:N	2.55	0.40
1:C:183:ARG:HG2	1:C:195:ARG:O	2.21	0.40
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.87	0.40
1:G:239:VAL:HG23	1:G:309:ALA:C	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:VAL:HB	1:H:91:ILE:CG2	2.51	0.40
1:H:80:SER:O	1:H:111:ALA:HB2	2.20	0.40
1:H:84:TRP:HE3	1:H:89:ILE:HG13	1.85	0.40
1:A:202:ASN:ND2	1:C:279:VAL:CG2	2.84	0.40
1:A:206:THR:CG2	1:A:231:ARG:HG2	2.50	0.40
1:A:300:MET:HB2	1:C:226:ASN:HD22	1.80	0.40
1:A:76:ASN:OD1	1:A:81:LEU:HB2	2.21	0.40
1:D:106:GLY:C	1:D:108:HIS:H	2.23	0.40
1:D:157:PHE:HE1	1:D:242:LEU:HD23	1.85	0.40
1:D:153:CYS:HB2	1:D:289:SER:O	2.21	0.40
1:E:316:GLY:C	1:E:318:SER:N	2.72	0.40
1:E:91:ILE:HA	1:E:115:LYS:O	2.21	0.40
1:F:162:ASP:CA	1:F:167:ILE:HD13	2.51	0.40
1:F:183:ARG:HG3	1:F:196:ALA:HA	2.03	0.40
1:G:256:ASN:OD1	1:G:297:THR:HG21	2.20	0.40
1:H:11:ILE:HD11	3:H:401:NAD:N7N	2.36	0.40
1:H:133:ASN:HD22	1:H:133:ASN:C	2.23	0.40
1:H:70:ILE:H	1:H:70:ILE:HD13	1.87	0.40
1:D:191:ARG:HH22	2:I:61:GLU:CB	2.35	0.40
1:Q:242:LEU:O	1:Q:306:LYS:HA	2.21	0.40
1:A:198:ALA:HB1	1:A:201:LEU:HD12	2.01	0.40
1:A:236:ASN:O	1:A:237:VAL:HB	2.21	0.40
1:B:173:THR:HA	1:B:228:ILE:O	2.22	0.40
1:B:3:VAL:HG12	1:B:4:ALA:N	2.36	0.40
1:E:183:ARG:NH1	1:E:183:ARG:HA	2.36	0.40
1:G:255:VAL:HG12	1:G:259:PHE:CE2	2.57	0.40
1:G:137:TYR:CE2	1:G:328:VAL:HA	2.57	0.40
1:H:102:ARG:NH2	1:H:124:ASP:HB3	2.31	0.40
1:H:126:PRO:O	1:H:144:ILE:HB	2.21	0.40
1:H:243:VAL:HG22	1:H:306:LYS:HE3	2.02	0.40
1:O:176:HIS:O	1:O:231:ARG:HA	2.21	0.40
1:O:98:VAL:CG2	1:O:99:PHE:CE2	3.03	0.40
1:A:3:VAL:HG12	1:A:4:ALA:N	2.36	0.40
1:A:56:ASP:O	1:A:66:VAL:HA	2.21	0.40
1:B:100:VAL:HA	1:B:118:ILE:HD13	2.03	0.40
1:B:154:LEU:HD12	1:B:154:LEU:N	2.36	0.40
1:B:251:PHE:CE1	1:B:254:GLU:HB2	2.57	0.40
1:B:38:LYS:N	1:B:38:LYS:HD2	2.37	0.40
1:D:173:THR:HA	1:D:228:ILE:O	2.21	0.40
1:E:10:ARG:HB2	3:E:401:NAD:PN	2.61	0.40
1:E:165:PHE:CD1	1:E:248:LYS:HD3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:ALA:HB1	1:F:151:THR:HB	2.04	0.40
1:G:183:ARG:CZ	1:G:187:ALA:HB3	2.51	0.40
1:G:197:ARG:O	1:G:199:ALA:N	2.55	0.40
1:G:173:THR:OG1	1:G:228:ILE:CD1	2.70	0.40
1:G:74:VAL:HG23	1:G:75:SER:N	2.37	0.40
1:H:73:VAL:O	1:H:73:VAL:CG1	2.62	0.40
2:M:60:LEU:O	2:M:61:GLU:C	2.60	0.40
1:O:69:LYS:NZ	5:O:540:HOH:O	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:541:HOH:O	5:Q:541:HOH:O[2_665]	2.11	0.09

## 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	334/337 (99%)	272 (81%)	54 (16%)	8 (2%)	7	17
1	B	334/337 (99%)	267 (80%)	55 (16%)	12 (4%)	4	9
1	C	334/337 (99%)	281 (84%)	44 (13%)	9 (3%)	6	15
1	D	334/337 (99%)	247 (74%)	63 (19%)	24 (7%)	1	1
1	E	334/337 (99%)	248 (74%)	58 (17%)	28 (8%)	1	1
1	F	334/337 (99%)	250 (75%)	64 (19%)	20 (6%)	2	3
1	G	335/337 (99%)	270 (81%)	47 (14%)	18 (5%)	2	4
1	H	333/337 (99%)	250 (75%)	51 (15%)	32 (10%)	1	0
1	O	335/337 (99%)	303 (90%)	29 (9%)	3 (1%)	20	46
1	Q	334/337 (99%)	294 (88%)	32 (10%)	8 (2%)	7	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	20/82 (24%)	19 (95%)	1 (5%)	0	100	100
2	J	19/82 (23%)	15 (79%)	3 (16%)	1 (5%)	2	4
2	K	19/82 (23%)	16 (84%)	1 (5%)	2 (10%)	0	0
2	L	17/82 (21%)	12 (71%)	4 (24%)	1 (6%)	2	3
2	M	20/82 (24%)	16 (80%)	3 (15%)	1 (5%)	2	4
2	N	17/82 (21%)	9 (53%)	7 (41%)	1 (6%)	2	3
All	All	3453/3862 (89%)	2769 (80%)	516 (15%)	168 (5%)	2	5

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ASP
1	B	221	LEU
1	D	22	ASP
1	D	199	ALA
1	D	210	ALA
1	E	0	LYS
1	E	20	ARG
1	E	177	SER
1	E	186	ASP
1	E	199	ALA
1	E	237	VAL
1	E	302	ASP
1	E	313	ASN
1	F	130	VAL
1	G	130	VAL
1	G	132	VAL
1	G	198	ALA
1	H	56	ASP
1	H	89	ILE
1	H	124	ASP
1	H	130	VAL
1	H	199	ALA
1	Q	33	THR
1	B	166	GLY
1	B	233	PRO
1	B	237	VAL
1	B	263	ALA
1	C	134	ALA
1	C	186	ASP

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Mol	Chain	Res	Type
1	C	237	VAL
1	D	55	ALA
1	D	72	GLN
1	D	130	VAL
1	D	180	GLY
1	D	200	ALA
1	D	313	ASN
1	E	33	THR
1	E	43	LEU
1	E	55	ALA
1	E	61	GLU
1	E	63	ALA
1	E	94	GLU
1	E	139	HIS
1	E	200	ALA
1	E	219	PRO
1	E	252	ALA
1	E	280	SER
1	F	8	PHE
1	F	132	VAL
1	F	135	ASP
1	F	248	LYS
1	F	331	ASN
1	G	135	ASP
1	G	154	LEU
1	G	163	GLN
1	G	166	GLY
1	G	233	PRO
1	G	281	VAL
1	G	295	SER
1	H	10	ARG
1	H	61	GLU
1	H	105	ALA
1	H	133	ASN
1	H	139	HIS
1	H	180	GLY
1	H	200	ALA
1	H	237	VAL
2	K	74	ARG
2	N	74	ARG
1	O	237	VAL
1	Q	1	LEU

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Mol	Chain	Res	Type
1	Q	111	ALA
1	Q	124	ASP
1	A	105	ALA
1	B	253	GLU
1	C	47	ASP
1	C	166	GLY
1	C	198	ALA
1	C	282	ASP
1	D	80	SER
1	D	146	ASN
1	D	155	ALA
1	D	193	LEU
1	D	237	VAL
1	D	289	SER
1	E	111	ALA
1	E	136	ALA
1	E	281	VAL
1	F	69	LYS
1	F	156	PRO
1	F	165	PHE
1	F	226	ASN
1	F	257	ALA
1	G	102	ARG
1	G	191	ARG
1	G	211	ALA
1	G	223	GLY
1	H	55	ALA
1	H	136	ALA
1	H	233	PRO
2	K	59	PRO
1	O	186	ASP
1	Q	237	VAL
1	A	110	GLU
1	A	237	VAL
1	B	193	LEU
1	B	198	ALA
1	B	223	GLY
1	D	125	ILE
1	E	142	PRO
1	E	317	TYR
1	F	62	THR
1	F	186	ASP

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Mol	Chain	Res	Type
1	F	223	GLY
1	F	252	ALA
1	F	253	GLU
1	F	258	ALA
1	G	237	VAL
1	H	52	ILE
1	H	86	GLU
1	H	142	PRO
1	H	146	ASN
1	H	178	TYR
2	J	74	ARG
1	Q	136	ALA
1	A	69	LYS
1	B	220	ASN
1	D	2	LYS
1	D	8	PHE
1	D	255	VAL
1	D	302	ASP
1	E	18(A)	TRP
1	E	28	ILE
1	E	233	PRO
1	F	237	VAL
1	G	155	ALA
1	G	226	ASN
1	H	67	ASP
1	H	87	LEU
1	H	147	ALA
1	H	163	GLN
1	H	211	ALA
1	H	282	ASP
1	A	38	LYS
1	A	83	PRO
1	A	233	PRO
1	B	94	GLU
1	C	233	PRO
1	D	54	ASP
1	D	233	PRO
1	E	56	ASP
1	F	24	PRO
1	H	79	PRO
1	H	82	LEU
1	Q	233	PRO

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Mol	Chain	Res	Type
1	Q	302	ASP
1	D	168	ILE
1	G	180	GLY
1	H	126	PRO
1	H	132	VAL
1	O	166	GLY
1	D	9	GLY
2	L	58	ASP
1	B	219	PRO
1	F	233	PRO
2	M	58	ASP
1	C	27	ILE
1	H	235	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/279 (100%)	260 (93%)	19 (7%)	18	41
1	B	279/279 (100%)	259 (93%)	20 (7%)	17	39
1	C	279/279 (100%)	255 (91%)	24 (9%)	12	28
1	D	279/279 (100%)	255 (91%)	24 (9%)	12	28
1	E	278/279 (100%)	255 (92%)	23 (8%)	13	30
1	F	279/279 (100%)	259 (93%)	20 (7%)	17	39
1	G	279/279 (100%)	261 (94%)	18 (6%)	20	44
1	H	278/279 (100%)	265 (95%)	13 (5%)	30	60
1	O	279/279 (100%)	260 (93%)	19 (7%)	18	41
1	Q	279/279 (100%)	266 (95%)	13 (5%)	30	60
2	I	22/65 (34%)	19 (86%)	3 (14%)	4	10
2	J	21/65 (32%)	21 (100%)	0	100	100
2	K	21/65 (32%)	19 (90%)	2 (10%)	10	23
2	L	18/65 (28%)	10 (56%)	8 (44%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	22/65 (34%)	22 (100%)	0	100	100
2	N	19/65 (29%)	19 (100%)	0	100	100
All	All	2911/3180 (92%)	2705 (93%)	206 (7%)	17	39

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	LYS
1	A	2	LYS
1	A	8	PHE
1	A	27	ILE
1	A	28	ILE
1	A	33	THR
1	A	69	LYS
1	A	74	VAL
1	A	76	ASN
1	A	84	TRP
1	A	133	ASN
1	A	164	LYS
1	A	171	THR
1	A	207	SER
1	A	239	VAL
1	A	240	VAL
1	A	245	GLN
1	A	280	SER
1	A	290	THR
1	B	38	LYS
1	B	84	TRP
1	B	91	ILE
1	B	94	GLU
1	B	103	GLU
1	B	117	ILE
1	B	133	ASN
1	B	135	ASP
1	B	152	ASN
1	B	157	PHE
1	B	163	GLN
1	B	172	MET
1	B	175	THR
1	B	178	TYR
1	B	191	ARG

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Mol	Chain	Res	Type
1	B	220	ASN
1	B	271	LEU
1	B	279	VAL
1	B	290	THR
1	B	311	TYR
1	C	14	ASN
1	C	16	LEU
1	C	21	LYS
1	C	25	LEU
1	C	61	GLU
1	C	65	SER
1	C	70	ILE
1	C	76	ASN
1	C	84	TRP
1	C	91	ILE
1	C	94	GLU
1	C	133	ASN
1	C	141	GLU
1	C	152	ASN
1	C	169	LYS
1	C	171	THR
1	C	203	ILE
1	C	208	THR
1	C	228	ILE
1	C	266	GLU
1	C	290	THR
1	C	295	SER
1	C	313	ASN
1	C	330	ASN
1	D	8	PHE
1	D	21	LYS
1	D	27	ILE
1	D	28	ILE
1	D	39	GLN
1	D	58	LYS
1	D	62	THR
1	D	67	ASP
1	D	84	TRP
1	D	87	LEU
1	D	124	ASP
1	D	152	ASN
1	D	169	LYS

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Mol	Chain	Res	Type
1	D	172	MET
1	D	178	TYR
1	D	191	ARG
1	D	201	LEU
1	D	202	ASN
1	D	220	ASN
1	D	228	ILE
1	D	234	THR
1	D	238	SER
1	D	245	GLN
1	D	261	ASP
1	E	5	ILE
1	E	28	ILE
1	E	37	VAL
1	E	38	LYS
1	E	56	ASP
1	E	58	LYS
1	E	61	GLU
1	E	67	ASP
1	E	70	ILE
1	E	84	TRP
1	E	87	LEU
1	E	133	ASN
1	E	144	ILE
1	E	163	GLN
1	E	172	MET
1	E	173	THR
1	E	178	TYR
1	E	179	THR
1	E	226	ASN
1	E	251	PHE
1	E	256	ASN
1	E	296	LEU
1	E	300	MET
1	F	1	LEU
1	F	8	PHE
1	F	14	ASN
1	F	18	CYS
1	F	21	LYS
1	F	84	TRP
1	F	94	GLU
1	F	122(A)	LYS

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Mol	Chain	Res	Type
1	F	124	ASP
1	F	127	THR
1	F	133	ASN
1	F	141	GLU
1	F	164	LYS
1	F	172	MET
1	F	178	TYR
1	F	228	ILE
1	F	274	CYS
1	F	290	THR
1	F	300	MET
1	F	302	ASP
1	G	23	SER
1	G	25	LEU
1	G	28	ILE
1	G	72	GLN
1	G	85	LYS
1	G	87	LEU
1	G	130	VAL
1	G	133	ASN
1	G	148	SER
1	G	169	LYS
1	G	205	PRO
1	G	242	LEU
1	G	253	GLU
1	G	256	ASN
1	G	264	GLU
1	G	291	THR
1	G	311	TYR
1	G	313	ASN
1	H	56	ASP
1	H	58	LYS
1	H	70	ILE
1	H	72	GLN
1	H	76	ASN
1	H	91	ILE
1	H	133	ASN
1	H	144	ILE
1	H	164	LYS
1	H	178	TYR
1	H	201	LEU
1	H	206	THR

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Mol	Chain	Res	Type
1	H	295	SER
2	I	58	ASP
2	I	74	ARG
2	I	77	ASP
2	K	67	ASN
2	K	69	GLU
2	L	55	ASP
2	L	58	ASP
2	L	61	GLU
2	L	62	GLU
2	L	63	TYR
2	L	65	LYS
2	L	70	THR
2	L	71	ASN
1	O	14	ASN
1	O	27	ILE
1	O	39	GLN
1	O	56	ASP
1	O	58	LYS
1	O	61	GLU
1	O	62	THR
1	O	74	VAL
1	O	75	SER
1	O	84	TRP
1	O	91	ILE
1	O	103	GLU
1	O	133	ASN
1	O	135	ASP
1	O	154	LEU
1	O	191	ARG
1	O	247	SER
1	O	265	LYS
1	O	268	LYS
1	Q	16	LEU
1	Q	74	VAL
1	Q	76	ASN
1	Q	84	TRP
1	Q	103	GLU
1	Q	124	ASP
1	Q	133	ASN
1	Q	140	ASP
1	Q	141	GLU

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Mol	Chain	Res	Type
1	Q	164	LYS
1	Q	290	THR
1	Q	323	ASP
1	Q	331	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	78	ASN
1	A	133	ASN
1	A	146	ASN
1	A	152	ASN
1	A	163	GLN
1	A	202	ASN
1	A	256	ASN
1	A	330	ASN
1	B	133	ASN
1	B	146	ASN
1	B	152	ASN
1	B	202	ASN
1	B	220	ASN
1	B	256	ASN
1	B	330	ASN
1	C	14	ASN
1	C	133	ASN
1	C	152	ASN
1	C	163	GLN
1	C	202	ASN
1	C	226	ASN
1	C	256	ASN
1	C	330	ASN
1	D	39	GLN
1	D	42	HIS
1	D	78	ASN
1	D	133	ASN
1	D	146	ASN
1	D	152	ASN
1	D	202	ASN
1	D	245	GLN
1	D	256	ASN
1	D	319	GLN

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Mol	Chain	Res	Type
1	D	330	ASN
1	D	331	ASN
1	E	39	GLN
1	E	76	ASN
1	E	133	ASN
1	E	146	ASN
1	E	152	ASN
1	E	330	ASN
1	F	14	ASN
1	F	18(B)	HIS
1	F	42	HIS
1	F	133	ASN
1	F	139	HIS
1	F	152	ASN
1	F	163	GLN
1	F	202	ASN
1	F	226	ASN
1	F	256	ASN
1	F	330	ASN
1	G	6	ASN
1	G	72	GLN
1	G	133	ASN
1	G	152	ASN
1	G	202	ASN
1	G	226	ASN
1	G	330	ASN
1	G	331	ASN
1	H	39	GLN
1	H	72	GLN
1	H	133	ASN
1	H	139	HIS
1	H	152	ASN
1	H	202	ASN
1	H	226	ASN
1	H	245	GLN
1	H	256	ASN
1	H	330	ASN
2	I	78	ASN
2	J	78	ASN
2	K	78	ASN
2	M	78	ASN
1	O	6	ASN

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Mol	Chain	Res	Type
1	O	39	GLN
1	O	72	GLN
1	O	133	ASN
1	O	152	ASN
1	O	202	ASN
1	O	256	ASN
1	Q	76	ASN
1	Q	133	ASN
1	Q	146	ASN
1	Q	152	ASN
1	Q	163	GLN
1	Q	202	ASN
1	Q	226	ASN
1	Q	256	ASN
1	Q	330	ASN
1	Q	331	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

38 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAD	A	401	-	41,48,48	1.43	7 (17%)	43,73,73	1.87	13 (30%)
4	SO4	A	402	-	4,4,4	0.34	0	6,6,6	0.17	0
4	SO4	A	403	-	4,4,4	0.36	0	6,6,6	0.10	0
4	SO4	A	404	-	4,4,4	0.34	0	6,6,6	0.18	0
4	SO4	A	405	-	4,4,4	0.39	0	6,6,6	0.08	0
4	SO4	A	406	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	A	407	-	4,4,4	0.29	0	6,6,6	0.13	0
4	SO4	A	408	-	4,4,4	0.31	0	6,6,6	0.06	0
3	NAD	B	401	-	41,48,48	1.57	8 (19%)	43,73,73	1.82	11 (25%)
4	SO4	B	402	-	4,4,4	0.32	0	6,6,6	0.14	0
4	SO4	B	403	-	4,4,4	0.35	0	6,6,6	0.15	0
3	NAD	C	401	-	41,48,48	1.54	6 (14%)	43,73,73	1.79	11 (25%)
4	SO4	C	402	-	4,4,4	0.35	0	6,6,6	0.12	0
4	SO4	C	403	-	4,4,4	0.36	0	6,6,6	0.17	0
4	SO4	C	404	-	4,4,4	0.34	0	6,6,6	0.15	0
4	SO4	C	405	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	C	406	-	4,4,4	0.32	0	6,6,6	0.21	0
3	NAD	D	401	-	41,48,48	1.41	7 (17%)	43,73,73	1.98	12 (27%)
4	SO4	D	402	-	4,4,4	0.33	0	6,6,6	0.14	0
3	NAD	E	401	-	41,48,48	1.38	7 (17%)	43,73,73	1.95	12 (27%)
4	SO4	E	402	-	4,4,4	0.30	0	6,6,6	0.05	0
4	SO4	E	403	-	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	E	404	-	4,4,4	0.36	0	6,6,6	0.09	0
3	NAD	F	401	-	41,48,48	1.55	6 (14%)	43,73,73	1.92	12 (27%)
4	SO4	F	402	-	4,4,4	0.29	0	6,6,6	0.18	0
4	SO4	F	403	-	4,4,4	0.29	0	6,6,6	0.12	0
3	NAD	G	401	-	41,48,48	1.55	8 (19%)	43,73,73	1.87	11 (25%)
4	SO4	G	402	-	4,4,4	0.30	0	6,6,6	0.12	0
3	NAD	H	401	-	41,48,48	1.42	5 (12%)	43,73,73	1.91	12 (27%)
4	SO4	H	402	-	4,4,4	0.42	0	6,6,6	0.09	0
3	NAD	O	401	-	41,48,48	1.37	6 (14%)	43,73,73	1.86	12 (27%)
4	SO4	O	402	-	4,4,4	0.30	0	6,6,6	0.13	0
4	SO4	O	403	-	4,4,4	0.30	0	6,6,6	0.12	0
3	NAD	Q	401	-	41,48,48	1.62	7 (17%)	43,73,73	1.79	10 (23%)
4	SO4	Q	402	-	4,4,4	0.39	0	6,6,6	0.14	0
4	SO4	Q	403	-	4,4,4	0.27	0	6,6,6	0.07	0
4	SO4	Q	404	-	4,4,4	0.41	0	6,6,6	0.13	0
4	SO4	Q	405	-	4,4,4	0.40	0	6,6,6	0.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	401	-	-	0/22/62/62	0/5/5/5
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	SO4	A	403	-	-	0/0/0/0	0/0/0/0
4	SO4	A	404	-	-	0/0/0/0	0/0/0/0
4	SO4	A	405	-	-	0/0/0/0	0/0/0/0
4	SO4	A	406	-	-	0/0/0/0	0/0/0/0
4	SO4	A	407	-	-	0/0/0/0	0/0/0/0
4	SO4	A	408	-	-	0/0/0/0	0/0/0/0
3	NAD	B	401	-	-	0/22/62/62	0/5/5/5
4	SO4	B	402	-	-	0/0/0/0	0/0/0/0
4	SO4	B	403	-	-	0/0/0/0	0/0/0/0
3	NAD	C	401	-	-	0/22/62/62	0/5/5/5
4	SO4	C	402	-	-	0/0/0/0	0/0/0/0
4	SO4	C	403	-	-	0/0/0/0	0/0/0/0
4	SO4	C	404	-	-	0/0/0/0	0/0/0/0
4	SO4	C	405	-	-	0/0/0/0	0/0/0/0
4	SO4	C	406	-	-	0/0/0/0	0/0/0/0
3	NAD	D	401	-	-	0/22/62/62	0/5/5/5
4	SO4	D	402	-	-	0/0/0/0	0/0/0/0
3	NAD	E	401	-	-	0/22/62/62	0/5/5/5
4	SO4	E	402	-	-	0/0/0/0	0/0/0/0
4	SO4	E	403	-	-	0/0/0/0	0/0/0/0
4	SO4	E	404	-	-	0/0/0/0	0/0/0/0
3	NAD	F	401	-	-	0/22/62/62	0/5/5/5
4	SO4	F	402	-	-	0/0/0/0	0/0/0/0
4	SO4	F	403	-	-	0/0/0/0	0/0/0/0
3	NAD	G	401	-	-	0/22/62/62	0/5/5/5
4	SO4	G	402	-	-	0/0/0/0	0/0/0/0
3	NAD	H	401	-	-	0/22/62/62	0/5/5/5
4	SO4	H	402	-	-	0/0/0/0	0/0/0/0
3	NAD	O	401	-	-	0/22/62/62	0/5/5/5
4	SO4	O	402	-	-	0/0/0/0	0/0/0/0
4	SO4	O	403	-	-	0/0/0/0	0/0/0/0
3	NAD	Q	401	-	-	0/22/62/62	0/5/5/5
4	SO4	Q	402	-	-	0/0/0/0	0/0/0/0
4	SO4	Q	403	-	-	0/0/0/0	0/0/0/0
4	SO4	Q	404	-	-	0/0/0/0	0/0/0/0
4	SO4	Q	405	-	-	0/0/0/0	0/0/0/0

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	NAD	C2B-C1B	-2.48	1.49	1.53
3	O	401	NAD	C2A-N1A	2.01	1.37	1.33
3	B	401	NAD	C2A-N3A	2.01	1.35	1.32
3	E	401	NAD	C2A-N1A	2.01	1.37	1.33
3	E	401	NAD	O3D-C3D	2.05	1.47	1.43
3	G	401	NAD	C5N-C4N	2.06	1.42	1.38
3	B	401	NAD	C4A-N3A	2.06	1.38	1.35
3	C	401	NAD	O3D-C3D	2.10	1.47	1.43
3	Q	401	NAD	O5B-C5B	2.11	1.53	1.44
3	E	401	NAD	O5B-C5B	2.13	1.53	1.44
3	O	401	NAD	C3D-C4D	2.13	1.58	1.53
3	D	401	NAD	C2A-N1A	2.13	1.37	1.33
3	Q	401	NAD	O3D-C3D	2.17	1.47	1.43
3	F	401	NAD	C4A-N3A	2.17	1.38	1.35
3	O	401	NAD	C5N-C4N	2.18	1.43	1.38
3	G	401	NAD	O3D-C3D	2.20	1.48	1.43
3	B	401	NAD	C5N-C4N	2.22	1.43	1.38
3	D	401	NAD	O4B-C1B	2.22	1.44	1.41
3	A	401	NAD	C2A-N3A	2.24	1.35	1.32
3	A	401	NAD	C5N-C4N	2.26	1.43	1.38
3	A	401	NAD	O3D-C3D	2.27	1.48	1.43
3	B	401	NAD	O5B-C5B	2.27	1.53	1.44
3	F	401	NAD	O4B-C1B	2.27	1.44	1.41
3	D	401	NAD	C2A-N3A	2.28	1.36	1.32
3	G	401	NAD	O5B-C5B	2.29	1.53	1.44
3	C	401	NAD	C5N-C4N	2.31	1.43	1.38
3	Q	401	NAD	C2A-N3A	2.38	1.36	1.32
3	H	401	NAD	C4A-N3A	2.51	1.39	1.35
3	B	401	NAD	O4B-C1B	2.52	1.44	1.41
3	G	401	NAD	C4A-N3A	2.53	1.39	1.35
3	A	401	NAD	C4A-N3A	2.56	1.39	1.35
3	D	401	NAD	C4N-C3N	2.58	1.43	1.39
3	H	401	NAD	O4B-C1B	2.68	1.45	1.41
3	E	401	NAD	C4A-N3A	2.72	1.39	1.35
3	E	401	NAD	C4N-C3N	2.77	1.43	1.39
3	D	401	NAD	C3N-C7N	2.80	1.54	1.50
3	O	401	NAD	C4N-C3N	2.83	1.44	1.39
3	A	401	NAD	C4N-C3N	2.83	1.44	1.39
3	C	401	NAD	O4B-C1B	2.91	1.45	1.41
3	F	401	NAD	C4N-C3N	2.91	1.44	1.39
3	Q	401	NAD	O4B-C1B	2.96	1.45	1.41
3	H	401	NAD	C4N-C3N	3.00	1.44	1.39
3	O	401	NAD	C3N-C7N	3.02	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	401	NAD	O4B-C1B	3.10	1.45	1.41
3	F	401	NAD	C6N-N1N	3.17	1.43	1.35
3	G	401	NAD	C4N-C3N	3.35	1.44	1.39
3	E	401	NAD	C6N-N1N	3.37	1.44	1.35
3	B	401	NAD	C4N-C3N	3.38	1.44	1.39
3	A	401	NAD	C3N-C7N	3.41	1.55	1.50
3	Q	401	NAD	C6N-N1N	3.46	1.44	1.35
3	G	401	NAD	C6N-N1N	3.47	1.44	1.35
3	D	401	NAD	C4A-N3A	3.47	1.40	1.35
3	E	401	NAD	C3N-C7N	3.47	1.55	1.50
3	B	401	NAD	C6N-N1N	3.53	1.44	1.35
3	D	401	NAD	C6N-N1N	3.57	1.44	1.35
3	A	401	NAD	C6N-N1N	3.59	1.44	1.35
3	C	401	NAD	C4N-C3N	3.63	1.45	1.39
3	O	401	NAD	C6N-N1N	3.64	1.44	1.35
3	H	401	NAD	C6N-N1N	3.64	1.44	1.35
3	Q	401	NAD	C4N-C3N	3.64	1.45	1.39
3	C	401	NAD	C6N-N1N	3.84	1.45	1.35
3	H	401	NAD	C3N-C7N	3.96	1.56	1.50
3	C	401	NAD	C3N-C7N	4.61	1.57	1.50
3	G	401	NAD	C3N-C7N	4.75	1.57	1.50
3	B	401	NAD	C3N-C7N	5.30	1.58	1.50
3	Q	401	NAD	C3N-C7N	5.42	1.59	1.50
3	F	401	NAD	C3N-C7N	5.74	1.59	1.50

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAD	C5N-C6N-N1N	-5.38	112.13	120.40
3	D	401	NAD	C5N-C6N-N1N	-5.34	112.19	120.40
3	O	401	NAD	C5N-C6N-N1N	-5.34	112.20	120.40
3	C	401	NAD	C5N-C6N-N1N	-5.25	112.34	120.40
3	B	401	NAD	C5N-C6N-N1N	-5.23	112.37	120.40
3	F	401	NAD	C5N-C6N-N1N	-5.22	112.38	120.40
3	E	401	NAD	C5N-C6N-N1N	-5.15	112.48	120.40
3	G	401	NAD	C5N-C6N-N1N	-5.08	112.59	120.40
3	H	401	NAD	C5N-C6N-N1N	-4.97	112.76	120.40
3	Q	401	NAD	C5N-C6N-N1N	-4.82	112.99	120.40
3	H	401	NAD	C4N-C3N-C7N	-4.07	110.25	121.07
3	E	401	NAD	C4N-C3N-C7N	-4.05	110.31	121.07
3	D	401	NAD	C4N-C3N-C7N	-3.99	110.47	121.07
3	D	401	NAD	C3N-C2N-N1N	-3.87	116.53	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	NAD	C4N-C3N-C7N	-3.72	111.18	121.07
3	G	401	NAD	C4N-C3N-C7N	-3.71	111.21	121.07
3	O	401	NAD	C4N-C3N-C7N	-3.55	111.62	121.07
3	A	401	NAD	C4N-C3N-C7N	-3.54	111.66	121.07
3	B	401	NAD	C4N-C3N-C7N	-3.45	111.90	121.07
3	H	401	NAD	C3N-C2N-N1N	-3.45	116.96	120.43
3	Q	401	NAD	C4N-C3N-C7N	-3.39	112.06	121.07
3	O	401	NAD	C5N-C4N-C3N	-3.33	116.43	120.35
3	C	401	NAD	C4N-C3N-C7N	-3.31	112.28	121.07
3	C	401	NAD	O3D-C3D-C4D	-3.30	101.44	111.09
3	E	401	NAD	C3N-C2N-N1N	-3.30	117.11	120.43
3	G	401	NAD	C3N-C2N-N1N	-3.09	117.32	120.43
3	F	401	NAD	C3N-C2N-N1N	-3.08	117.32	120.43
3	A	401	NAD	C5N-C4N-C3N	-3.06	116.75	120.35
3	D	401	NAD	O3D-C3D-C4D	-3.05	102.18	111.09
3	E	401	NAD	C5N-C4N-C3N	-3.05	116.76	120.35
3	B	401	NAD	C5N-C4N-C3N	-3.02	116.79	120.35
3	C	401	NAD	C3N-C2N-N1N	-3.01	117.40	120.43
3	H	401	NAD	C5N-C4N-C3N	-2.99	116.83	120.35
3	Q	401	NAD	C5N-C4N-C3N	-2.96	116.87	120.35
3	G	401	NAD	C5N-C4N-C3N	-2.92	116.92	120.35
3	E	401	NAD	O7N-C7N-C3N	-2.91	116.22	119.62
3	D	401	NAD	C5N-C4N-C3N	-2.87	116.97	120.35
3	F	401	NAD	C5N-C4N-C3N	-2.84	117.01	120.35
3	D	401	NAD	O7N-C7N-C3N	-2.77	116.38	119.62
3	A	401	NAD	C3N-C2N-N1N	-2.74	117.67	120.43
3	Q	401	NAD	C3N-C2N-N1N	-2.74	117.67	120.43
3	E	401	NAD	O3D-C3D-C4D	-2.65	103.35	111.09
3	A	401	NAD	O3D-C3D-C4D	-2.62	103.42	111.09
3	C	401	NAD	C5N-C4N-C3N	-2.56	117.33	120.35
3	E	401	NAD	C1B-N9A-C4A	-2.55	122.23	126.64
3	O	401	NAD	N3A-C2A-N1A	-2.52	126.66	128.86
3	H	401	NAD	O7N-C7N-C3N	-2.51	116.69	119.62
3	B	401	NAD	C3N-C2N-N1N	-2.49	117.92	120.43
3	G	401	NAD	O3D-C3D-C4D	-2.47	103.88	111.09
3	F	401	NAD	O3D-C3D-C4D	-2.46	103.89	111.09
3	G	401	NAD	O7N-C7N-C3N	-2.44	116.77	119.62
3	O	401	NAD	O7N-C7N-C3N	-2.42	116.79	119.62
3	O	401	NAD	O5B-C5B-C4B	-2.40	100.48	109.00
3	Q	401	NAD	O3D-C3D-C4D	-2.36	104.19	111.09
3	F	401	NAD	C1B-N9A-C4A	-2.29	122.67	126.64
3	O	401	NAD	C3N-C2N-N1N	-2.24	118.17	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	NAD	N3A-C2A-N1A	-2.24	126.90	128.86
3	F	401	NAD	N3A-C2A-N1A	-2.24	126.91	128.86
3	H	401	NAD	O3D-C3D-C4D	-2.22	104.60	111.09
3	A	401	NAD	N3A-C2A-N1A	-2.22	126.92	128.86
3	B	401	NAD	O3D-C3D-C4D	-2.21	104.64	111.09
3	A	401	NAD	O5B-C5B-C4B	-2.20	101.19	109.00
3	H	401	NAD	N3A-C2A-N1A	-2.19	126.95	128.86
3	A	401	NAD	O7N-C7N-C3N	-2.17	117.08	119.62
3	D	401	NAD	N3A-C2A-N1A	-2.13	127.00	128.86
3	C	401	NAD	N3A-C2A-N1A	-2.08	127.05	128.86
3	B	401	NAD	C1B-N9A-C4A	-2.04	123.11	126.64
3	O	401	NAD	C1B-N9A-C4A	-2.02	123.14	126.64
3	C	401	NAD	O5B-C5B-C4B	-2.02	101.85	109.00
3	A	401	NAD	C4D-O4D-C1D	2.08	111.98	109.77
3	F	401	NAD	C2N-C3N-C4N	2.13	120.69	118.26
3	B	401	NAD	C5A-C6A-N6A	2.26	125.09	120.47
3	Q	401	NAD	C4D-O4D-C1D	2.34	112.26	109.77
3	H	401	NAD	C4D-O4D-C1D	2.44	112.36	109.77
3	C	401	NAD	C2N-C3N-C4N	2.44	121.04	118.26
3	B	401	NAD	C2N-C3N-C4N	2.46	121.07	118.26
3	O	401	NAD	C2N-C3N-C7N	2.47	126.53	119.34
3	Q	401	NAD	C2N-C3N-C4N	2.48	121.08	118.26
3	F	401	NAD	C4D-O4D-C1D	2.48	112.41	109.77
3	C	401	NAD	C2N-C3N-C7N	2.52	126.68	119.34
3	Q	401	NAD	C2N-C3N-C7N	2.58	126.86	119.34
3	A	401	NAD	C2N-C3N-C7N	2.60	126.91	119.34
3	G	401	NAD	C2N-C3N-C4N	2.63	121.26	118.26
3	B	401	NAD	C2N-C3N-C7N	2.65	127.03	119.34
3	G	401	NAD	C4D-O4D-C1D	2.66	112.60	109.77
3	D	401	NAD	C2N-C3N-C7N	2.77	127.41	119.34
3	A	401	NAD	C2N-C3N-C4N	2.78	121.43	118.26
3	D	401	NAD	C4D-O4D-C1D	2.79	112.74	109.77
3	G	401	NAD	C2N-C3N-C7N	2.82	127.53	119.34
3	C	401	NAD	C3N-C7N-N7N	2.96	121.16	117.77
3	E	401	NAD	C2N-C3N-C7N	2.98	128.00	119.34
3	H	401	NAD	C2N-C3N-C7N	2.98	128.00	119.34
3	E	401	NAD	C2N-C3N-C4N	3.01	121.69	118.26
3	F	401	NAD	C2N-C3N-C7N	3.02	128.13	119.34
3	A	401	NAD	C3N-C7N-N7N	3.03	121.23	117.77
3	H	401	NAD	C2N-C3N-C4N	3.06	121.75	118.26
3	O	401	NAD	C2N-C3N-C4N	3.14	121.85	118.26
3	D	401	NAD	C3N-C7N-N7N	3.29	121.53	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	401	NAD	C3N-C7N-N7N	3.34	121.59	117.77
3	D	401	NAD	C2N-C3N-C4N	3.38	122.12	118.26
3	F	401	NAD	C3N-C7N-N7N	3.61	121.89	117.77
3	H	401	NAD	C3N-C7N-N7N	3.70	122.00	117.77
3	D	401	NAD	C6N-C5N-C4N	3.71	125.03	119.44
3	B	401	NAD	C3N-C7N-N7N	3.74	122.04	117.77
3	C	401	NAD	C6N-C5N-C4N	3.74	125.09	119.44
3	O	401	NAD	C3N-C7N-N7N	3.75	122.06	117.77
3	E	401	NAD	C3N-C7N-N7N	3.77	122.08	117.77
3	Q	401	NAD	C6N-C5N-C4N	3.80	125.17	119.44
3	O	401	NAD	C6N-C5N-C4N	3.81	125.18	119.44
3	G	401	NAD	C6N-C5N-C4N	3.83	125.22	119.44
3	B	401	NAD	C6N-C5N-C4N	3.84	125.24	119.44
3	E	401	NAD	C6N-C5N-C4N	3.85	125.24	119.44
3	H	401	NAD	C6N-C5N-C4N	3.86	125.26	119.44
3	A	401	NAD	C6N-C5N-C4N	3.94	125.38	119.44
3	G	401	NAD	C3N-C7N-N7N	4.18	122.54	117.77
3	F	401	NAD	C6N-C5N-C4N	4.30	125.92	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAD	3	0
4	A	406	SO4	1	0
3	B	401	NAD	1	0
4	B	402	SO4	1	0
3	C	401	NAD	2	0
4	C	404	SO4	1	0
3	D	401	NAD	6	0
4	D	402	SO4	1	0
3	E	401	NAD	5	0
4	E	402	SO4	1	0
4	E	403	SO4	1	0
3	F	401	NAD	6	0
3	G	401	NAD	1	0
3	H	401	NAD	13	0
3	Q	401	NAD	1	0
4	Q	404	SO4	1	0



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	336/337 (99%)	0.24	4 (1%) 79 80	32, 50, 71, 80	0
1	B	336/337 (99%)	0.46	9 (2%) 55 55	37, 58, 81, 95	0
1	C	336/337 (99%)	0.53	15 (4%) 34 32	39, 57, 76, 95	0
1	D	336/337 (99%)	0.70	22 (6%) 20 17	50, 80, 97, 116	0
1	E	336/337 (99%)	1.73	121 (36%) 0 0	62, 87, 108, 113	0
1	F	336/337 (99%)	1.07	60 (17%) 2 1	46, 83, 102, 118	0
1	G	337/337 (100%)	0.70	23 (6%) 18 16	38, 66, 89, 98	0
1	H	335/337 (99%)	0.88	36 (10%) 7 5	51, 83, 109, 115	0
1	O	337/337 (100%)	0.31	0 100 100	17, 31, 47, 54	0
1	Q	336/337 (99%)	0.19	0 100 100	20, 37, 54, 74	0
2	I	22/82 (26%)	0.96	3 (13%) 3 2	76, 81, 88, 93	0
2	J	21/82 (25%)	0.69	2 (9%) 9 7	66, 75, 86, 91	0
2	K	21/82 (25%)	4.37	21 (100%) 0 0	9, 24, 31, 31	21 (100%)
2	L	19/82 (23%)	4.71	19 (100%) 0 0	38, 51, 70, 76	19 (100%)
2	M	22/82 (26%)	1.30	3 (13%) 3 2	64, 76, 98, 107	0
2	N	19/82 (23%)	2.25	8 (42%) 0 0	67, 81, 85, 86	19 (100%)
All	All	3485/3862 (90%)	0.74	346 (9%) 8 6	9, 64, 99, 118	59 (1%)

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	LEU	9.1
2	L	55	ASP	7.7
1	E	129	VAL	7.6
2	K	58	ASP	6.8
2	L	58	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
2	K	70	THR	6.5
2	K	64	CYS	6.4
1	E	229	ALA	6.4
1	E	64	ILE	6.0
2	N	70	THR	6.0
1	E	44	LEU	5.9
1	E	1	LEU	5.6
2	K	59	PRO	5.6
1	E	15	PHE	5.6
1	E	28	ILE	5.6
2	K	67	ASN	5.4
1	G	269	GLY	5.2
1	E	79	PRO	5.2
2	L	60	LEU	5.2
2	K	61	GLU	5.1
2	L	59	PRO	5.1
2	L	63	TYR	5.1
2	L	64	CYS	5.1
2	K	73	CYS	5.0
2	L	56	GLY	5.0
1	E	300	MET	5.0
2	K	66	ASP	4.9
2	M	57	SER	4.9
2	K	63	TYR	4.9
2	K	68	PRO	4.8
1	E	37	VAL	4.7
2	N	68	PRO	4.7
2	L	65	LYS	4.7
2	K	62	GLU	4.7
2	L	57	SER	4.7
1	D	95	GLY	4.7
1	E	29	ALA	4.6
1	H	143	ILE	4.6
1	E	-1	ALA	4.6
2	L	66	ASP	4.5
1	F	267	LEU	4.5
2	L	61	GLU	4.5
2	L	70	THR	4.4
2	K	60	LEU	4.4
1	H	57	VAL	4.4
2	L	73	CYS	4.4
1	E	328	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	212	LYS	4.3
1	E	116	VAL	4.3
1	H	89	ILE	4.3
1	E	55	ALA	4.3
1	E	118	ILE	4.3
2	L	71	ASN	4.3
1	E	143	ILE	4.3
1	H	225	LEU	4.2
1	F	333	LYS	4.2
2	L	62	GLU	4.2
1	E	100	VAL	4.2
1	C	332	TRP	4.2
1	E	53	PHE	4.1
1	E	114	LYS	4.1
1	E	187	ALA	4.1
1	E	98	VAL	4.1
1	E	157	PHE	4.0
1	E	158	VAL	4.0
2	K	76	TYR	4.0
1	G	305	VAL	3.9
1	E	258	ALA	3.9
1	A	187	ALA	3.8
1	H	187	ALA	3.8
1	E	171	THR	3.8
2	L	69	GLU	3.8
1	C	265	LYS	3.8
1	E	154	LEU	3.8
2	L	72	GLU	3.7
1	E	21	LYS	3.7
1	C	37	VAL	3.6
1	E	292	ILE	3.6
2	L	67	ASN	3.6
1	E	310	TRP	3.6
1	F	315	TRP	3.6
1	E	324	LEU	3.6
1	E	179	THR	3.6
2	N	60	LEU	3.5
1	H	84	TRP	3.5
2	K	69	GLU	3.5
1	G	274	CYS	3.5
1	G	244	VAL	3.5
2	K	78	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	218	LEU	3.5
1	F	278	LEU	3.4
1	D	329	ALA	3.4
2	M	78	ASN	3.4
1	F	87	LEU	3.4
1	E	57	VAL	3.4
1	E	273	VAL	3.4
1	H	227	GLY	3.4
1	E	193	LEU	3.4
1	H	44	LEU	3.4
1	F	43	LEU	3.3
1	B	271	LEU	3.3
1	E	66	VAL	3.3
1	H	119	THR	3.3
1	E	325	ALA	3.3
1	E	7	GLY	3.3
1	E	270	ILE	3.3
1	F	296	LEU	3.3
1	D	332	TRP	3.2
1	E	267	LEU	3.2
1	D	128	TYR	3.2
2	N	59	PRO	3.2
1	F	237	VAL	3.2
1	E	109	ILE	3.2
1	E	48	SER	3.2
2	N	69	GLU	3.2
1	E	204	VAL	3.2
1	F	322	VAL	3.2
1	G	254	GLU	3.2
1	G	130	VAL	3.2
1	E	322	VAL	3.1
2	K	65	LYS	3.1
1	E	317	TYR	3.1
2	L	68	PRO	3.1
1	E	228	ILE	3.1
1	H	228	ILE	3.1
1	F	299	VAL	3.1
1	G	-1	ALA	3.1
1	G	199	ALA	3.0
1	F	10	ARG	3.0
1	E	108	HIS	3.0
1	C	333	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	24	PRO	3.0
1	E	203	ILE	3.0
1	E	56	ASP	3.0
1	F	268	LYS	3.0
1	E	18(A)	TRP	3.0
1	D	136	ALA	2.9
1	F	5	ILE	2.9
1	F	28	ILE	2.9
1	E	284	ARG	2.9
2	K	72	GLU	2.9
2	K	77	ASP	2.9
1	F	259	PHE	2.9
1	G	273	VAL	2.9
1	H	157	PHE	2.9
1	H	128	TYR	2.9
1	G	225	LEU	2.8
1	E	138	SER	2.8
1	C	88	GLY	2.8
1	D	53	PHE	2.8
1	E	230	LEU	2.8
1	F	56	ASP	2.8
1	H	24	PRO	2.8
1	D	137	TYR	2.8
1	F	332	TRP	2.8
1	E	50	LEU	2.8
1	E	33	THR	2.8
1	F	46	TYR	2.8
1	F	164	LYS	2.8
1	G	160	VAL	2.7
1	H	25	LEU	2.7
1	H	193	LEU	2.7
1	F	252	ALA	2.7
1	F	27	ILE	2.7
1	F	128	TYR	2.7
1	E	74	VAL	2.7
1	E	81	LEU	2.7
1	E	161	LEU	2.7
1	F	330	ASN	2.7
1	F	288	PHE	2.7
1	F	167	ILE	2.7
1	E	101	ASP	2.7
1	F	312	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	84	TRP	2.7
1	E	206	THR	2.7
1	E	196	ALA	2.7
1	E	250	THR	2.7
1	E	211	ALA	2.6
1	F	286	SER	2.6
1	E	183	ARG	2.6
1	C	91	ILE	2.6
1	F	153	CYS	2.6
1	F	261	ASP	2.6
1	G	247	SER	2.6
1	E	84	TRP	2.6
1	H	28	ILE	2.6
1	E	78	ASN	2.6
1	E	140	ASP	2.6
1	C	84	TRP	2.6
1	D	263	ALA	2.6
1	F	57	VAL	2.6
2	K	71	ASN	2.6
1	E	243	VAL	2.6
1	E	329	ALA	2.6
2	N	61	GLU	2.6
2	K	74	ARG	2.6
1	D	119	THR	2.5
1	F	52	ILE	2.5
1	H	117	ILE	2.5
1	E	61	GLU	2.5
1	F	311	TYR	2.5
1	C	5	ILE	2.5
1	E	85	LYS	2.5
1	E	259	PHE	2.5
1	E	5	ILE	2.5
1	F	89	ILE	2.5
1	H	147	ALA	2.5
1	E	311	TYR	2.5
1	E	31	ASN	2.5
1	E	27	ILE	2.5
1	E	43	LEU	2.5
1	F	266	GLU	2.5
1	D	100	VAL	2.5
1	E	255	VAL	2.5
1	E	321	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	262	SER	2.5
1	C	87	LEU	2.5
1	D	130	VAL	2.5
1	B	333	LYS	2.4
1	E	127	THR	2.4
1	D	89	ILE	2.4
1	D	267	LEU	2.4
1	E	320	ARG	2.4
1	G	170	GLY	2.4
1	E	59	PRO	2.4
1	A	89	ILE	2.4
1	E	278	LEU	2.4
1	F	307	VAL	2.4
1	C	25	LEU	2.4
1	D	161	LEU	2.4
1	F	292	ILE	2.4
1	C	322	VAL	2.4
1	F	108	HIS	2.4
1	H	332	TRP	2.4
1	H	188	SER	2.4
2	I	57	SER	2.4
1	E	298	MET	2.4
1	B	263	ALA	2.4
1	E	283	PHE	2.4
1	A	139	HIS	2.4
1	H	83	PRO	2.4
1	E	327	ILE	2.4
1	E	80	SER	2.3
1	F	111	ALA	2.3
1	F	155	ALA	2.3
1	E	128	TYR	2.3
1	F	45	LYS	2.3
1	F	269	GLY	2.3
1	H	191	ARG	2.3
1	D	118	ILE	2.3
1	H	108	HIS	2.3
1	E	14	ASN	2.3
1	E	76	ASN	2.3
2	K	75	THR	2.3
1	H	116	VAL	2.3
1	E	314	GLU	2.3
1	H	185	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	96	THR	2.3
1	B	292	ILE	2.3
1	B	161	LEU	2.3
1	D	184	LEU	2.3
1	G	161	LEU	2.3
1	C	89	ILE	2.3
1	H	64	ILE	2.3
1	D	129	VAL	2.3
1	F	273	VAL	2.3
1	F	326	ASP	2.3
1	F	112	GLY	2.3
1	H	315	TRP	2.3
1	E	182	GLN	2.3
1	G	304	MET	2.3
1	E	275	ASP	2.3
1	G	128	TYR	2.2
1	C	36	GLY	2.2
1	H	144	ILE	2.2
1	G	201	LEU	2.2
1	G	216	LEU	2.2
1	G	221	LEU	2.2
2	J	60	LEU	2.2
1	E	99	PHE	2.2
1	E	30	ILE	2.2
1	F	70	ILE	2.2
1	E	231	ARG	2.2
1	D	170	GLY	2.2
1	D	28	ILE	2.2
1	E	246	VAL	2.2
1	H	42	HIS	2.2
1	G	163	GLN	2.2
1	H	27	ILE	2.2
1	H	63	ALA	2.2
1	E	117	ILE	2.2
1	E	245	GLN	2.2
1	E	67	ASP	2.2
1	B	251	PHE	2.2
1	E	89	ILE	2.2
1	F	130	VAL	2.2
2	M	60	LEU	2.2
1	E	58	LYS	2.1
2	J	76	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	240	VAL	2.1
1	E	144	ILE	2.1
1	E	216	LEU	2.1
2	N	76	TYR	2.1
1	E	82	LEU	2.1
1	F	271	LEU	2.1
1	E	241	ASP	2.1
1	F	300	MET	2.1
1	F	146	ASN	2.1
1	B	139	HIS	2.1
1	B	230	LEU	2.1
1	G	270	ILE	2.1
1	E	287	ASP	2.1
2	I	60	LEU	2.1
2	I	77	ASP	2.1
1	E	249	LYS	2.1
1	G	129	VAL	2.1
1	H	186	ASP	2.1
1	H	113	ALA	2.1
1	E	39	GLN	2.1
1	E	106	GLY	2.1
1	F	270	ILE	2.1
1	A	206	THR	2.1
2	N	66	ASP	2.1
1	E	92	VAL	2.1
1	E	46	TYR	2.1
1	F	0	LYS	2.1
1	H	60	SER	2.1
1	D	117	ILE	2.1
1	D	325	ALA	2.1
1	C	50	LEU	2.0
1	D	154	LEU	2.0
1	G	268	LYS	2.0
1	C	137	TYR	2.0
1	E	12	GLY	2.0
1	E	318	SER	2.0
1	F	82	LEU	2.0
1	F	242	LEU	2.0
1	H	221	LEU	2.0
1	F	8	PHE	2.0
1	H	218	LEU	2.0
1	E	77	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	255	VAL	2.0
1	E	210	ALA	2.0
1	F	88	GLY	2.0
1	E	151	THR	2.0
1	F	154	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	O	403	5/5	0.88	0.41	15.99	48,48,49,49	5
4	SO4	B	403	5/5	0.80	0.49	10.31	61,62,63,64	5
4	SO4	O	402	5/5	0.92	0.29	6.06	38,38,40,41	5
4	SO4	Q	404	5/5	0.79	0.33	5.15	50,51,52,52	5
4	SO4	Q	403	5/5	0.90	0.25	5.03	50,50,50,52	5
4	SO4	Q	405	5/5	0.86	0.29	4.71	80,81,81,82	5
4	SO4	A	407	5/5	0.91	0.27	3.46	46,47,48,48	5
4	SO4	C	406	5/5	0.89	0.25	2.17	42,43,44,45	5
4	SO4	G	402	5/5	0.80	0.33	1.64	54,54,55,55	5
4	SO4	H	402	5/5	0.90	0.23	1.07	90,91,91,92	0
4	SO4	C	404	5/5	0.91	0.22	0.92	69,69,70,70	5
4	SO4	D	402	5/5	0.80	0.25	0.74	44,45,46,47	5
4	SO4	A	405	5/5	0.96	0.20	0.62	75,75,76,76	0
3	NAD	B	401	44/44	0.96	0.20	0.11	52,57,59,60	0
3	NAD	D	401	44/44	0.91	0.24	0.05	70,76,81,81	0
4	SO4	A	403	5/5	0.95	0.16	0.05	82,82,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAD	Q	401	44/44	0.97	0.21	-0.02	32,39,41,44	0
4	SO4	C	405	5/5	0.92	0.21	-0.18	68,69,70,70	5
3	NAD	H	401	44/44	0.87	0.25	-0.25	100,103,104,104	0
3	NAD	G	401	44/44	0.97	0.20	-0.28	40,47,52,54	0
3	NAD	A	401	44/44	0.95	0.18	-0.42	51,54,57,60	0
3	NAD	O	401	44/44	0.98	0.21	-0.46	20,26,30,33	0
4	SO4	F	403	5/5	0.92	0.16	-0.69	78,79,79,80	5
3	NAD	C	401	44/44	0.96	0.18	-0.80	50,55,58,60	0
3	NAD	E	401	44/44	0.92	0.25	-0.87	87,90,92,94	0
3	NAD	F	401	44/44	0.94	0.20	-0.89	70,73,76,77	0
4	SO4	C	403	5/5	0.98	0.15	-1.50	70,70,71,71	0
4	SO4	A	404	5/5	0.98	0.18	-1.56	58,60,60,61	0
4	SO4	E	403	5/5	0.84	0.20	-1.83	58,58,59,60	5
4	SO4	E	404	5/5	0.91	0.11	-2.73	72,72,73,74	5
4	SO4	A	406	5/5	0.95	0.15	-	63,64,65,65	5
4	SO4	A	408	5/5	0.84	0.24	-	69,70,70,71	5
4	SO4	F	402	5/5	0.94	0.19	-	89,89,90,90	0
4	SO4	Q	402	5/5	0.96	0.20	-	80,80,80,81	0
4	SO4	A	402	5/5	0.98	0.19	-	74,74,75,76	0
4	SO4	E	402	5/5	0.89	0.27	-	79,80,81,81	5
4	SO4	B	402	5/5	0.86	0.23	-	52,52,53,53	5
4	SO4	C	402	5/5	0.95	0.20	-	85,86,87,87	0

## 6.5 Other polymers

There are no such residues in this entry.