



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:36 am GMT

PDB ID : 1JQK  
Title : Crystal structure of carbon monoxide dehydrogenase from Rhodospirillum rubrum  
Authors : Drennan, C.L.; Heo, J.; Sintchak, M.D.; Schreiter, E.; Ludden, P.W.  
Deposited on : 2001-08-07  
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

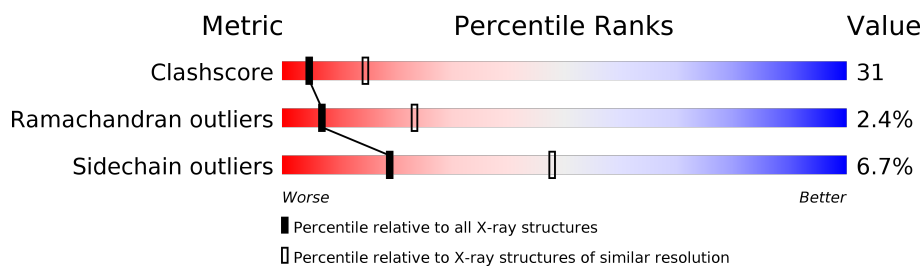
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	639	
1	B	639	
1	C	639	
1	D	639	
1	E	639	
1	F	639	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26898 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 carbon monoxide dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	S	0	0	0
			4461	2798	792	838	33			
1	B	610	Total	C	N	O	S	0	0	0
			4461	2798	792	838	33			
1	C	610	Total	C	N	O	S	0	0	0
			4461	2798	792	838	33			
1	D	610	Total	C	N	O	S	0	0	0
			4461	2798	792	838	33			
1	E	610	Total	C	N	O	S	0	0	0
			4461	2798	792	838	33			
1	F	610	Total	C	N	O	S	0	0	0
			4461	2798	792	838	33			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

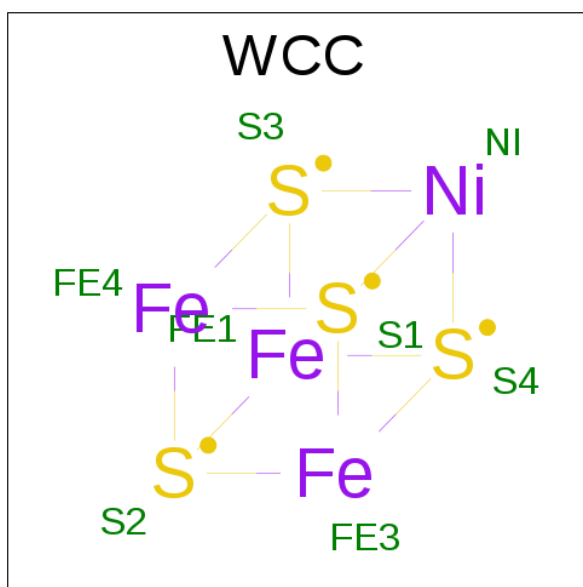
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(3)-NI(1)-S(4) CLUSTER (three-letter code: WCC) (formula: Fe<sub>3</sub>NiS<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			8	3	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			8	3	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			8	3	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			8	3	1	4		
4	E	1	Total	Fe	Ni	S	0	0
			8	3	1	4		
4	F	1	Total	Fe	Ni	S	0	0
			8	3	1	4		

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

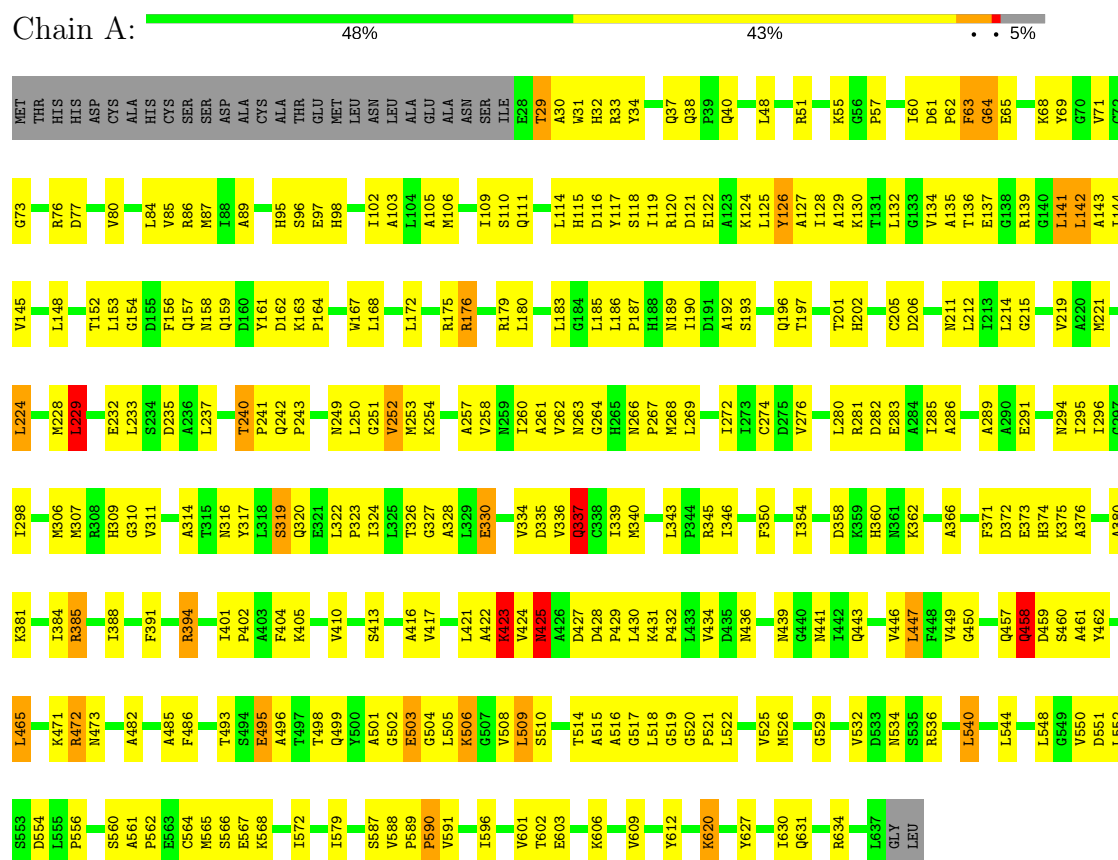
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	X	0	0
			1	1		
5	E	1	Total	X	0	0
			1	1		
5	B	1	Total	X	0	0
			1	1		
5	C	1	Total	X	0	0
			1	1		
5	A	1	Total	X	0	0
			1	1		
5	F	1	Total	X	0	0
			1	1		

### 3 Residue-property plots

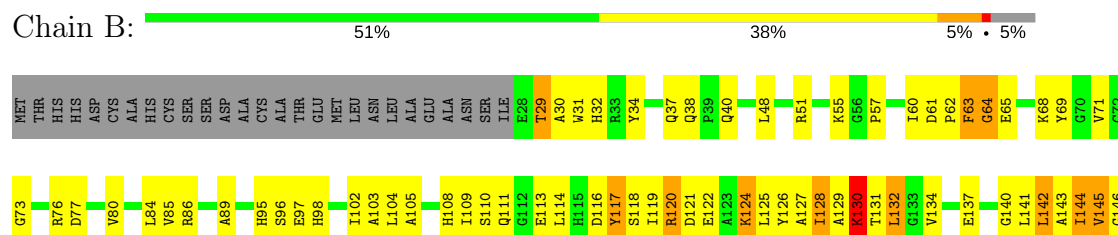
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

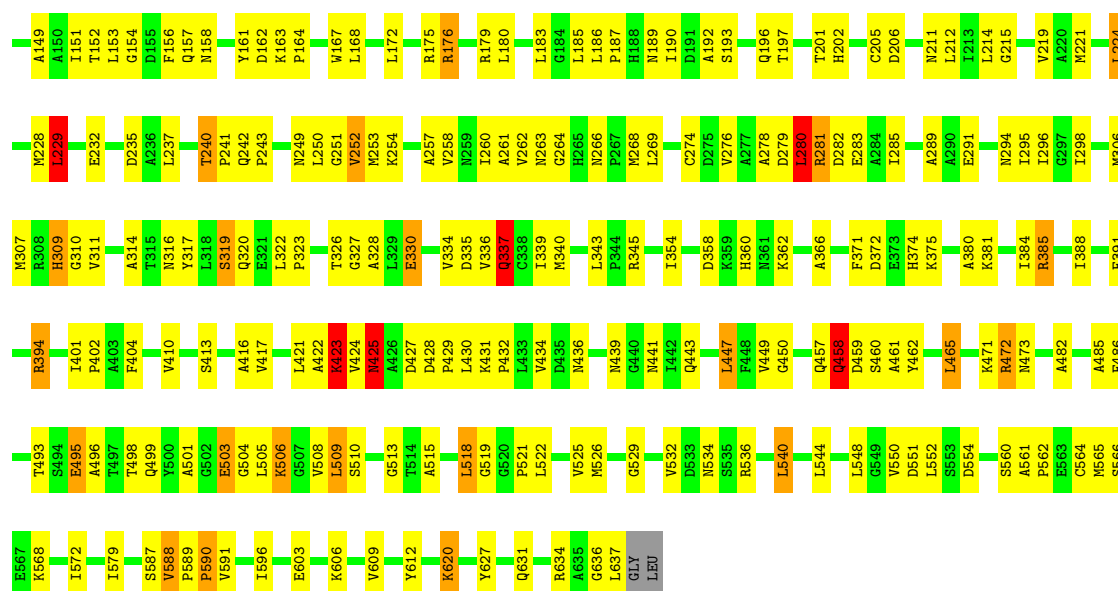
Note EDS was not executed.

- Molecule 1: carbon monoxide dehydrogenase



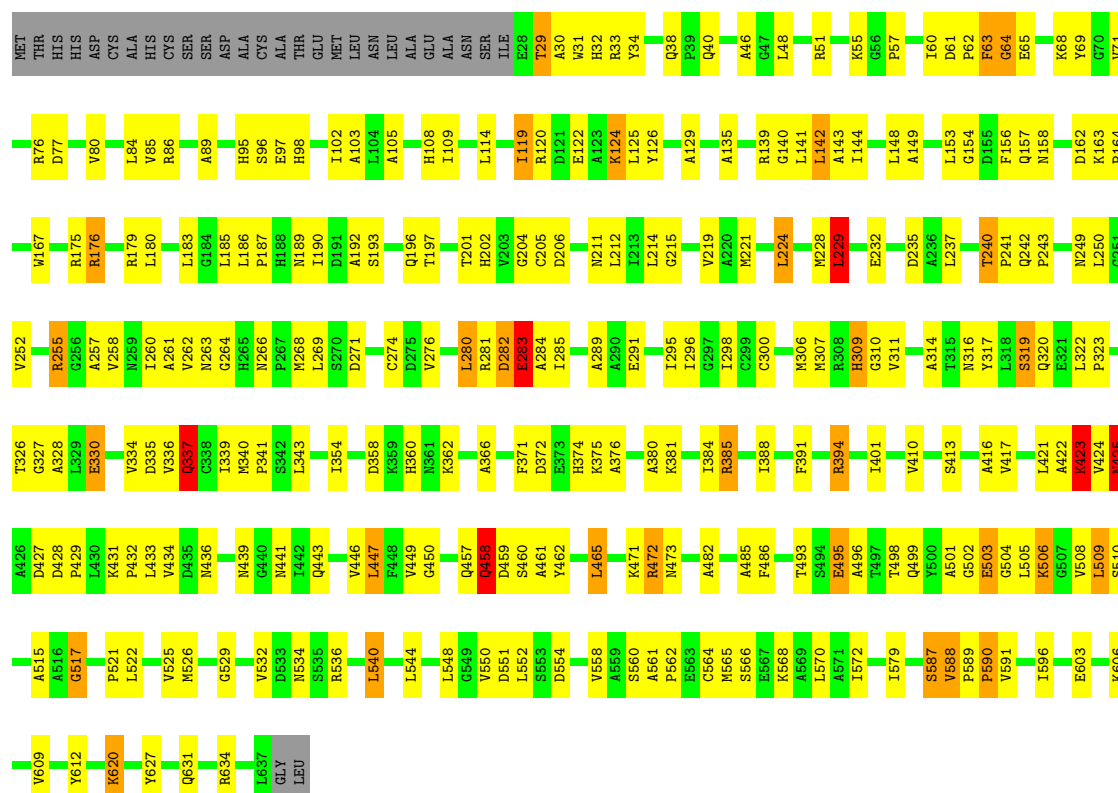
- Molecule 1: carbon monoxide dehydrogenase





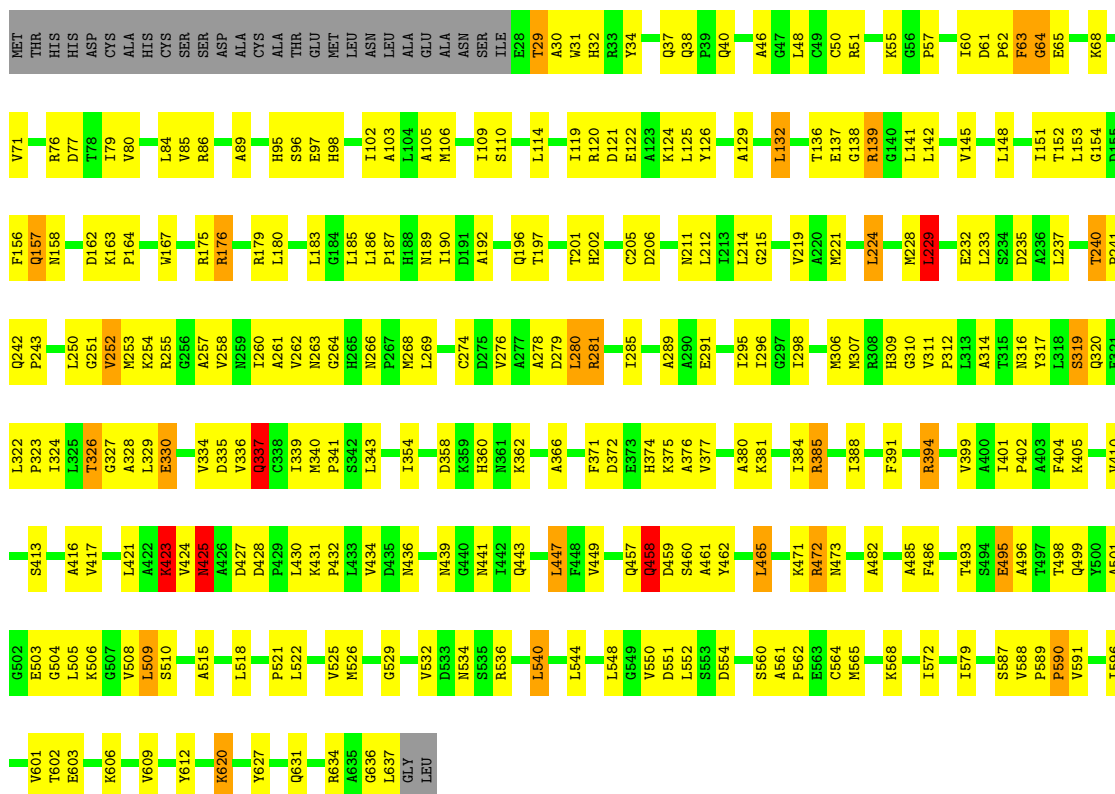
- Molecule 1: carbon monoxide dehydrogenase

Chain C:  54% 36% 5% • 5%



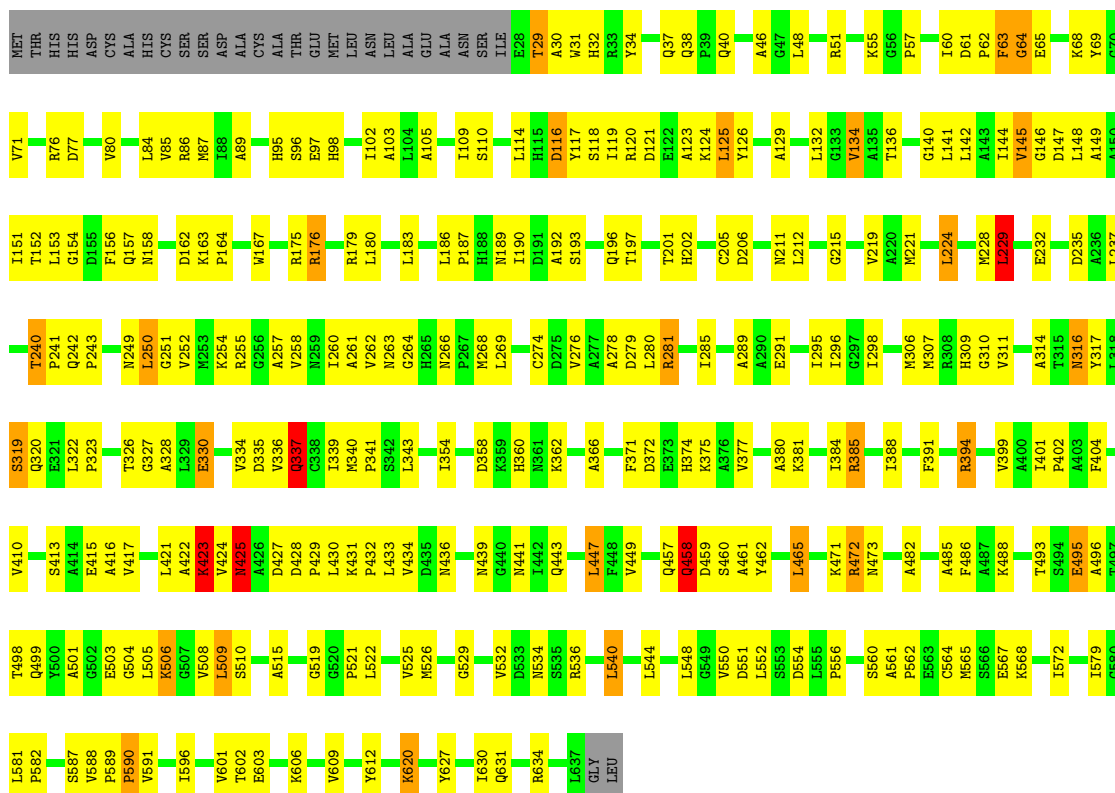
- Molecule 1: carbon monoxide dehydrogenase

Chain D:  53% 38% 5%



• Molecule 1: carbon monoxide dehydrogenase

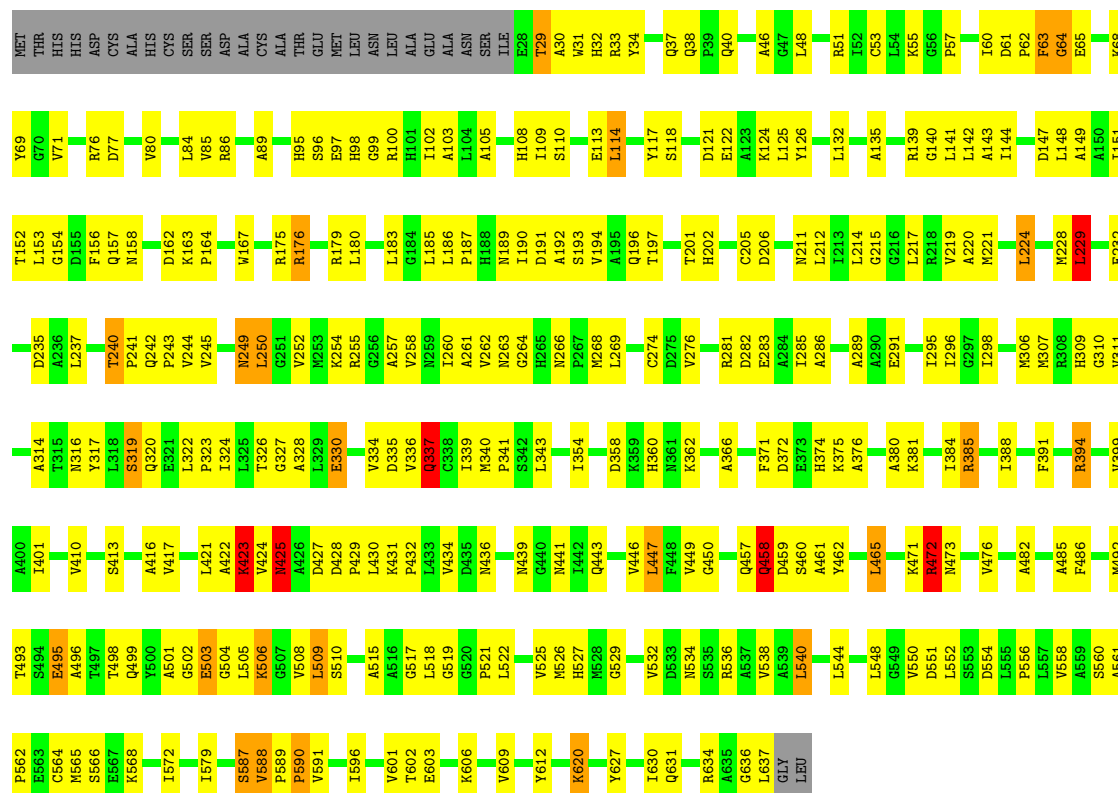
Chain E: 52% 38% 5%





- Molecule 1: carbon monoxide dehydrogenase

Chain F:  50% 41% . . 5%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.60Å 200.10Å 116.80Å 90.00° 111.50° 90.00°	Depositor
Resolution (Å)	100.00 – 2.80	Depositor
% Data completeness (in resolution range)	76.9 (100.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.257 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, SF4, FE2, WCC

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	0.35	0/4534	0.62	1/6161 (0.0%)
1	B	0.36	0/4534	0.63	1/6161 (0.0%)
1	C	0.40	0/4534	0.64	1/6161 (0.0%)
1	D	0.41	0/4534	0.64	1/6161 (0.0%)
1	E	0.41	0/4534	0.65	1/6161 (0.0%)
1	F	0.42	0/4534	0.65	1/6161 (0.0%)
All	All	0.39	0/27204	0.64	6/36966 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	229	LEU	CA-CB-CG	6.07	129.27	115.30
1	A	229	LEU	CA-CB-CG	5.67	128.35	115.30
1	D	229	LEU	CA-CB-CG	5.59	128.16	115.30
1	C	229	LEU	CA-CB-CG	5.47	127.89	115.30
1	F	229	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	229	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	126	TYR	Sidechain

## 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	4461	0	4529	311	0
1	B	4461	0	4529	341	0
1	C	4461	0	4529	262	0
1	D	4461	0	4528	267	0
1	E	4461	0	4528	273	0
1	F	4461	0	4528	280	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	16	0	0	0	0
3	B	8	0	0	0	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
3	E	16	0	0	0	0
3	F	8	0	0	0	0
4	A	8	0	0	1	0
4	B	8	0	0	1	0
4	C	8	0	0	1	0
4	D	8	0	0	0	0
4	E	8	0	0	0	0
4	F	8	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	26898	0	27171	1652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1652) 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:C:65:GLU:HA	1:C:68:LYS:HE2	1.34	1.09
1:D:65:GLU:HA	1:D:68:LYS:HE2	1.35	1.08
1:E:65:GLU:HA	1:E:68:LYS:HE2	1.34	1.08
1:A:65:GLU:HA	1:A:68:LYS:HE2	1.33	1.07
1:F:65:GLU:HA	1:F:68:LYS:HE2	1.34	1.06
1:B:65:GLU:HA	1:B:68:LYS:HE2	1.34	1.05
1:B:522:LEU:HD13	1:B:526:MET:HE3	1.41	1.02
1:D:141:LEU:HD12	1:D:142:LEU:HD12	1.39	1.01
1:B:132:LEU:HD22	1:B:151:ILE:HD13	1.40	1.01
1:F:334:VAL:HB	1:F:339:ILE:HD13	1.41	1.00
1:F:522:LEU:HD13	1:F:526:MET:HE3	1.40	1.00
1:C:522:LEU:HD13	1:C:526:MET:HE3	1.43	0.99
1:D:132:LEU:HD11	1:D:151:ILE:HG21	1.46	0.98
1:E:334:VAL:HB	1:E:339:ILE:HD13	1.45	0.98
1:B:127:ALA:HA	1:B:130:LYS:HZ3	1.27	0.98
1:E:255:ARG:HD3	1:E:399:VAL:HG11	1.45	0.97
1:A:110:SER:HA	1:A:142:LEU:HD22	1.46	0.97
1:A:522:LEU:HD13	1:A:526:MET:HE3	1.47	0.97
1:C:334:VAL:HB	1:C:339:ILE:HD13	1.45	0.97
1:B:334:VAL:HB	1:B:339:ILE:HD13	1.44	0.96
1:D:334:VAL:HB	1:D:339:ILE:HD13	1.48	0.96
1:D:522:LEU:HD13	1:D:526:MET:HE3	1.46	0.96
1:A:334:VAL:HB	1:A:339:ILE:HD13	1.43	0.95
1:A:119:ILE:HG12	1:A:141:LEU:HD21	1.45	0.93
1:E:522:LEU:HD13	1:E:526:MET:HE3	1.48	0.92
1:B:126:TYR:HA	1:B:129:ALA:HB3	1.53	0.90
1:A:254:LYS:HB2	1:A:257:ALA:HB3	1.52	0.89
1:B:63:PHE:CE2	1:F:62:PRO:HG3	2.08	0.89
1:B:254:LYS:HG3	1:B:257:ALA:HB3	1.53	0.88
1:B:110:SER:HB3	1:B:145:VAL:HG23	1.54	0.88
1:C:300:CYS:HG	2:C:801:FE2:FE	0.86	0.88
1:F:250:LEU:HD21	1:F:323:PRO:HG3	1.56	0.88
1:E:241:PRO:HG2	1:E:413:SER:HB3	1.57	0.87
1:A:122:GLU:OE2	1:A:141:LEU:HD13	1.74	0.87
1:D:255:ARG:NH2	1:D:399:VAL:HB	1.90	0.87
1:E:472:ARG:HB3	1:E:627:TYR:CE2	2.10	0.86
1:D:241:PRO:HG2	1:D:413:SER:HB3	1.56	0.86
1:A:241:PRO:HG2	1:A:413:SER:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:PRO:HG2	1:F:413:SER:HB3	1.59	0.85
1:A:620:LYS:HA	1:A:620:LYS:HE3	1.58	0.85
1:B:472:ARG:HB3	1:B:627:TYR:CE2	2.12	0.84
1:A:34:TYR:HA	1:B:71:VAL:HG22	1.58	0.84
1:A:472:ARG:HB3	1:A:627:TYR:CE2	2.12	0.84
1:B:241:PRO:HG2	1:B:413:SER:HB3	1.57	0.84
1:C:340:MET:O	1:C:343:LEU:HD23	1.78	0.84
1:A:211:ASN:ND2	1:B:362:LYS:HD2	1.92	0.84
1:C:241:PRO:HG2	1:C:413:SER:HB3	1.59	0.84
1:D:472:ARG:HB3	1:D:627:TYR:CE2	2.14	0.83
1:E:340:MET:O	1:E:343:LEU:HD23	1.78	0.83
1:F:472:ARG:HB3	1:F:627:TYR:CE2	2.14	0.83
1:C:472:ARG:HB3	1:C:627:TYR:CE2	2.13	0.83
1:B:620:LYS:HA	1:B:620:LYS:HE3	1.61	0.82
1:A:124:LYS:NZ	1:A:232:GLU:HA	1.94	0.82
1:F:29:THR:HG23	1:F:31:TRP:H	1.44	0.82
1:F:340:MET:O	1:F:343:LEU:HD23	1.79	0.82
1:A:362:LYS:HD2	1:B:211:ASN:ND2	1.95	0.82
1:F:620:LYS:HE3	1:F:620:LYS:HA	1.61	0.82
1:B:63:PHE:O	1:B:65:GLU:N	2.12	0.82
1:B:125:LEU:HD23	1:B:125:LEU:O	1.80	0.82
1:B:603:GLU:HA	1:B:606:LYS:HE2	1.62	0.82
1:B:63:PHE:HE2	1:F:62:PRO:HG3	1.45	0.82
1:B:372:ASP:HB3	1:B:375:LYS:HZ2	1.44	0.82
1:A:125:LEU:HA	1:A:128:ILE:HD12	1.62	0.81
1:C:29:THR:HG23	1:C:31:TRP:H	1.45	0.81
1:D:340:MET:O	1:D:343:LEU:HD23	1.80	0.81
1:D:620:LYS:HE3	1:D:620:LYS:HA	1.63	0.81
1:B:340:MET:O	1:B:343:LEU:HD23	1.78	0.81
1:C:55:LYS:HG3	1:D:565:MET:HG3	1.62	0.81
1:A:211:ASN:HD22	1:B:362:LYS:HD2	1.46	0.81
1:B:29:THR:HG23	1:B:31:TRP:H	1.44	0.81
1:C:603:GLU:HA	1:C:606:LYS:HE2	1.63	0.80
1:A:71:VAL:HG22	1:B:34:TYR:HA	1.62	0.80
1:B:457:GLN:HB2	1:B:460:SER:HB2	1.63	0.80
1:C:620:LYS:HA	1:C:620:LYS:HE3	1.62	0.80
1:A:29:THR:HG23	1:A:31:TRP:H	1.45	0.80
1:F:108:HIS:HB3	1:F:114:LEU:HD13	1.63	0.80
1:F:603:GLU:HA	1:F:606:LYS:HE2	1.64	0.80
1:B:126:TYR:OH	1:B:141:LEU:HD11	1.82	0.80
1:E:29:THR:HG23	1:E:31:TRP:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ASN:HA	1:C:439:ASN:HD21	1.46	0.79
1:A:65:GLU:HA	1:A:68:LYS:CE	2.12	0.79
1:B:119:ILE:HG22	1:B:120:ARG:N	1.97	0.79
1:F:65:GLU:HA	1:F:68:LYS:CE	2.11	0.79
1:A:603:GLU:HA	1:A:606:LYS:HE2	1.64	0.79
1:E:565:MET:HG3	1:F:55:LYS:HG3	1.62	0.79
1:D:252:VAL:HG21	1:D:312:PRO:HB2	1.64	0.79
1:D:603:GLU:HA	1:D:606:LYS:HE2	1.65	0.79
1:A:55:LYS:HG3	1:B:565:MET:HG3	1.63	0.79
1:F:457:GLN:HB2	1:F:460:SER:HB2	1.65	0.79
1:B:250:LEU:HD21	1:B:323:PRO:HG3	1.64	0.79
1:B:436:ASN:HA	1:B:439:ASN:HD21	1.48	0.79
1:B:127:ALA:HA	1:B:130:LYS:NZ	1.99	0.78
1:C:417:VAL:HG11	1:C:540:LEU:HD11	1.66	0.78
1:A:139:ARG:NH2	1:A:143:ALA:HB1	1.98	0.78
1:A:196:GLN:HG2	1:B:97:GLU:OE1	1.84	0.78
1:E:372:ASP:HB3	1:E:375:LYS:HZ2	1.49	0.78
1:C:63:PHE:O	1:C:65:GLU:N	2.15	0.78
1:E:65:GLU:HA	1:E:68:LYS:CE	2.12	0.78
1:C:65:GLU:HA	1:C:68:LYS:CE	2.12	0.78
1:C:457:GLN:HB2	1:C:460:SER:HB2	1.64	0.77
1:E:603:GLU:HA	1:E:606:LYS:HE2	1.65	0.77
1:E:63:PHE:O	1:E:65:GLU:N	2.14	0.77
1:C:565:MET:HG3	1:D:55:LYS:HG3	1.65	0.77
1:A:340:MET:O	1:A:343:LEU:HD23	1.83	0.77
1:A:457:GLN:HB2	1:A:460:SER:HB2	1.64	0.77
1:D:65:GLU:HA	1:D:68:LYS:CE	2.14	0.77
1:F:63:PHE:O	1:F:65:GLU:N	2.16	0.77
1:A:417:VAL:HG11	1:A:540:LEU:HD11	1.66	0.77
1:A:97:GLU:OE1	1:B:196:GLN:HG2	1.85	0.77
1:E:620:LYS:HE3	1:E:620:LYS:HA	1.65	0.77
1:A:127:ALA:O	1:A:130:LYS:HB3	1.85	0.77
1:B:141:LEU:HA	1:B:144:ILE:HD11	1.65	0.77
1:C:250:LEU:HD21	1:C:323:PRO:HG3	1.66	0.76
1:A:110:SER:HB3	1:A:145:VAL:HG12	1.65	0.76
1:E:457:GLN:HB2	1:E:460:SER:HB2	1.66	0.76
1:A:126:TYR:CE2	1:A:136:THR:HB	2.21	0.76
1:A:254:LYS:HD3	1:A:291:GLU:HB3	1.66	0.76
1:E:55:LYS:HG3	1:F:565:MET:HG3	1.67	0.76
1:B:254:LYS:HE3	1:B:294:ASN:HB2	1.68	0.76
1:D:29:THR:HG23	1:D:31:TRP:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:550:VAL:HG22	1:F:551:ASP:H	1.51	0.76
1:A:517:GLY:O	1:A:518:LEU:HD13	1.85	0.76
1:C:135:ALA:O	1:C:139:ARG:HD3	1.86	0.76
1:A:63:PHE:O	1:A:65:GLU:N	2.16	0.76
1:B:65:GLU:HA	1:B:68:LYS:CE	2.14	0.76
1:E:417:VAL:HG11	1:E:540:LEU:HD11	1.68	0.76
1:F:175:ARG:HH12	1:F:550:VAL:HA	1.51	0.76
1:F:493:THR:CG2	1:F:495:GLU:HG2	2.16	0.76
1:A:565:MET:HG3	1:B:55:LYS:HG3	1.67	0.75
1:A:436:ASN:HA	1:A:439:ASN:HD21	1.49	0.75
1:D:372:ASP:HB3	1:D:375:LYS:HZ2	1.51	0.75
1:F:124:LYS:HG2	1:F:235:ASP:HB3	1.65	0.75
1:F:372:ASP:HB3	1:F:375:LYS:HZ2	1.51	0.75
1:F:417:VAL:HG11	1:F:540:LEU:HD11	1.69	0.75
1:B:62:PRO:HG3	1:F:63:PHE:CE2	2.20	0.75
1:D:457:GLN:HB2	1:D:460:SER:HB2	1.68	0.75
1:D:63:PHE:O	1:D:65:GLU:N	2.16	0.75
1:B:141:LEU:O	1:B:144:ILE:HG12	1.86	0.75
1:B:110:SER:HB3	1:B:145:VAL:O	1.86	0.75
1:C:180:LEU:HB2	1:C:186:LEU:HD13	1.69	0.74
1:B:264:GLY:HA3	1:B:335:ASP:OD1	1.87	0.74
1:A:124:LYS:O	1:A:128:ILE:HG13	1.87	0.74
1:C:436:ASN:HA	1:C:439:ASN:ND2	2.03	0.74
1:F:462:TYR:HE2	1:F:562:PRO:HD2	1.53	0.74
1:D:462:TYR:HE2	1:D:562:PRO:HD2	1.52	0.74
1:F:175:ARG:NH1	1:F:550:VAL:HA	2.02	0.74
1:B:518:LEU:CD1	1:B:519:GLY:H	2.01	0.74
1:E:196:GLN:HG2	1:F:97:GLU:OE1	1.87	0.74
1:B:417:VAL:HG11	1:B:540:LEU:HD11	1.69	0.74
1:C:550:VAL:HG22	1:C:551:ASP:H	1.52	0.74
1:B:179:ARG:O	1:B:183:LEU:HD13	1.88	0.74
1:B:175:ARG:HH12	1:B:550:VAL:HA	1.53	0.74
1:F:336:VAL:HG12	1:F:337:GLN:HG2	1.69	0.73
1:A:175:ARG:NH1	1:A:550:VAL:HA	2.03	0.73
1:B:518:LEU:HD12	1:B:519:GLY:H	1.53	0.73
1:D:436:ASN:HA	1:D:439:ASN:HD21	1.53	0.73
1:E:132:LEU:HD12	1:E:148:LEU:CD2	2.18	0.73
1:A:336:VAL:HG12	1:A:337:GLN:HG2	1.70	0.73
1:B:129:ALA:HA	1:B:134:VAL:HG11	1.71	0.73
1:A:250:LEU:HD12	1:A:250:LEU:H	1.54	0.73
1:A:175:ARG:HH12	1:A:550:VAL:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:TYR:HE2	1:B:562:PRO:HD2	1.52	0.73
1:F:436:ASN:HA	1:F:439:ASN:HD21	1.53	0.73
1:B:436:ASN:HA	1:B:439:ASN:ND2	2.03	0.73
1:B:258:VAL:HG13	1:B:330:GLU:HG2	1.70	0.73
1:E:436:ASN:HA	1:E:439:ASN:HD21	1.53	0.73
1:A:362:LYS:HD2	1:B:211:ASN:HD22	1.54	0.73
1:A:372:ASP:HB3	1:A:375:LYS:HZ2	1.55	0.72
1:A:258:VAL:HG13	1:A:330:GLU:HG2	1.71	0.72
1:B:550:VAL:HG22	1:B:551:ASP:H	1.52	0.72
1:C:493:THR:CG2	1:C:495:GLU:HG2	2.19	0.72
1:E:462:TYR:HE2	1:E:562:PRO:HD2	1.55	0.72
1:F:258:VAL:HG13	1:F:330:GLU:HG2	1.71	0.72
1:A:436:ASN:HA	1:A:439:ASN:ND2	2.04	0.72
1:B:180:LEU:HB2	1:B:186:LEU:HD13	1.72	0.72
1:C:175:ARG:NH1	1:C:550:VAL:HA	2.04	0.72
1:D:550:VAL:HG22	1:D:551:ASP:H	1.55	0.72
1:E:97:GLU:OE1	1:F:196:GLN:HG2	1.89	0.72
1:A:264:GLY:HA3	1:A:335:ASP:OD1	1.90	0.72
1:A:493:THR:CG2	1:A:495:GLU:HG2	2.20	0.72
1:A:550:VAL:HG22	1:A:551:ASP:H	1.54	0.72
1:C:509:LEU:HD13	1:C:522:LEU:HB2	1.72	0.72
1:D:179:ARG:O	1:D:183:LEU:HD13	1.89	0.72
1:D:417:VAL:HG11	1:D:540:LEU:HD11	1.71	0.72
1:B:493:THR:CG2	1:B:495:GLU:HG2	2.20	0.71
1:C:264:GLY:HA3	1:C:335:ASP:OD1	1.89	0.71
1:E:175:ARG:HH12	1:E:550:VAL:HA	1.54	0.71
1:B:62:PRO:HG3	1:F:63:PHE:HE2	1.55	0.71
1:A:179:ARG:O	1:A:183:LEU:HD13	1.90	0.71
1:E:116:ASP:OD1	1:E:377:VAL:HG23	1.90	0.71
1:B:119:ILE:CG2	1:B:120:ARG:H	2.04	0.71
1:D:254:LYS:HB2	1:D:257:ALA:HB3	1.70	0.71
1:B:144:ILE:C	1:B:146:GLY:H	1.92	0.71
1:B:175:ARG:NH1	1:B:550:VAL:HA	2.04	0.71
1:D:175:ARG:HH12	1:D:550:VAL:HA	1.55	0.71
1:E:258:VAL:HG13	1:E:330:GLU:HG2	1.73	0.71
1:C:175:ARG:HH12	1:C:550:VAL:HA	1.53	0.71
1:C:421:LEU:O	1:C:424:VAL:HG12	1.91	0.71
1:C:71:VAL:HG22	1:D:34:TYR:HA	1.72	0.71
1:D:175:ARG:NH1	1:D:550:VAL:HA	2.04	0.71
1:E:175:ARG:NH1	1:E:550:VAL:HA	2.05	0.71
1:B:142:LEU:HA	1:B:145:VAL:HG22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:550:VAL:HG22	1:E:551:ASP:H	1.54	0.71
1:D:493:THR:CG2	1:D:495:GLU:HG2	2.20	0.71
1:E:264:GLY:HA3	1:E:335:ASP:OD1	1.91	0.71
1:E:509:LEU:HD13	1:E:522:LEU:HB2	1.73	0.71
1:A:180:LEU:HB2	1:A:186:LEU:HD13	1.72	0.70
1:E:180:LEU:HB2	1:E:186:LEU:HD13	1.73	0.70
1:B:421:LEU:O	1:B:424:VAL:HG12	1.91	0.70
1:E:34:TYR:HA	1:F:71:VAL:HG22	1.74	0.70
1:A:254:LYS:HD3	1:A:291:GLU:CB	2.22	0.70
1:C:97:GLU:OE1	1:D:196:GLN:HG2	1.91	0.70
1:F:493:THR:HG22	1:F:496:ALA:H	1.56	0.70
1:D:180:LEU:HB2	1:D:186:LEU:HD13	1.73	0.70
1:E:568:LYS:H	1:F:202:HIS:HE1	1.38	0.70
1:F:180:LEU:HB2	1:F:186:LEU:HD13	1.72	0.70
1:C:34:TYR:HA	1:D:71:VAL:HG22	1.72	0.70
1:A:472:ARG:HG2	1:A:472:ARG:HH11	1.56	0.69
1:C:120:ARG:NH2	1:C:271:ASP:OD1	2.25	0.69
1:D:224:LEU:HD11	1:D:579:ILE:HD11	1.74	0.69
1:F:509:LEU:HD13	1:F:522:LEU:HB2	1.73	0.69
1:C:372:ASP:HB3	1:C:375:LYS:HZ2	1.57	0.69
1:E:493:THR:CG2	1:E:495:GLU:HG2	2.22	0.69
1:A:202:HIS:HE1	1:B:568:LYS:H	1.40	0.69
1:E:436:ASN:HA	1:E:439:ASN:ND2	2.06	0.69
1:F:264:GLY:HA3	1:F:335:ASP:OD1	1.90	0.69
1:F:421:LEU:O	1:F:424:VAL:HG12	1.92	0.69
1:F:436:ASN:HA	1:F:439:ASN:ND2	2.07	0.69
1:B:224:LEU:HD11	1:B:579:ILE:HD11	1.73	0.69
1:B:509:LEU:HD13	1:B:522:LEU:HB2	1.75	0.69
1:D:436:ASN:HA	1:D:439:ASN:ND2	2.07	0.69
1:C:472:ARG:HH11	1:C:472:ARG:HG2	1.57	0.69
1:A:509:LEU:HD13	1:A:522:LEU:HB2	1.74	0.69
1:D:421:LEU:O	1:D:424:VAL:HG12	1.92	0.69
1:E:421:LEU:O	1:E:424:VAL:HG12	1.91	0.69
1:C:462:TYR:HE2	1:C:562:PRO:HD2	1.57	0.69
1:A:462:TYR:HE2	1:A:562:PRO:HD2	1.56	0.69
1:C:258:VAL:HG13	1:C:330:GLU:HG2	1.74	0.69
1:E:336:VAL:HG12	1:E:337:GLN:HG2	1.73	0.69
1:E:71:VAL:HG22	1:F:34:TYR:HA	1.75	0.69
1:E:140:GLY:O	1:E:142:LEU:N	2.25	0.68
1:F:249:ASN:O	1:F:252:VAL:HG23	1.93	0.68
1:A:421:LEU:O	1:A:424:VAL:HG12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:SER:CB	1:B:145:VAL:HG23	2.22	0.68
1:D:250:LEU:HD11	1:D:323:PRO:HG3	1.75	0.68
1:C:336:VAL:HG12	1:C:337:GLN:HG2	1.75	0.68
1:C:196:GLN:HG2	1:D:97:GLU:OE1	1.92	0.68
1:B:336:VAL:HG12	1:B:337:GLN:HG2	1.74	0.68
1:E:510:SER:HA	1:E:521:PRO:HB3	1.76	0.68
1:B:121:ASP:OD1	1:B:124:LYS:HB2	1.93	0.68
1:A:510:SER:HA	1:A:521:PRO:HB3	1.74	0.68
1:A:124:LYS:HZ1	1:A:232:GLU:HA	1.56	0.68
1:A:224:LEU:HD11	1:A:579:ILE:HD11	1.75	0.68
1:E:110:SER:HB3	1:E:145:VAL:CG2	2.24	0.67
1:D:258:VAL:HG13	1:D:330:GLU:HG2	1.74	0.67
1:D:264:GLY:HA3	1:D:335:ASP:OD1	1.93	0.67
1:C:249:ASN:O	1:C:252:VAL:HG22	1.94	0.67
1:D:141:LEU:HD12	1:D:142:LEU:CD1	2.18	0.67
1:E:278:ALA:O	1:E:281:ARG:HB3	1.94	0.67
1:D:125:LEU:HD12	1:D:148:LEU:HD12	1.75	0.67
1:D:509:LEU:HD13	1:D:522:LEU:HB2	1.76	0.67
1:A:493:THR:HG22	1:A:496:ALA:H	1.60	0.67
1:B:119:ILE:CG2	1:B:120:ARG:N	2.57	0.67
1:B:472:ARG:HG2	1:B:472:ARG:HH11	1.59	0.67
1:B:493:THR:HG22	1:B:496:ALA:H	1.60	0.67
1:F:179:ARG:O	1:F:183:LEU:HD13	1.95	0.67
1:F:443:GLN:HA	1:F:634:ARG:NH2	2.10	0.67
1:F:472:ARG:HH11	1:F:472:ARG:HG2	1.59	0.67
1:A:254:LYS:HB2	1:A:257:ALA:CB	2.24	0.67
1:B:128:ILE:HG21	1:B:232:GLU:HB3	1.76	0.67
1:C:493:THR:HG22	1:C:496:ALA:H	1.60	0.67
1:F:113:GLU:O	1:F:114:LEU:HB2	1.94	0.67
1:A:77:ASP:OD1	1:A:596:ILE:HD13	1.95	0.66
1:D:251:GLY:HA3	1:D:404:PHE:O	1.95	0.66
1:D:493:THR:HG22	1:D:496:ALA:H	1.60	0.66
1:C:202:HIS:HE1	1:D:568:LYS:H	1.41	0.66
1:B:126:TYR:O	1:B:130:LYS:HG2	1.94	0.66
1:C:215:GLY:O	1:C:219:VAL:HG23	1.94	0.66
1:B:129:ALA:CA	1:B:134:VAL:HG11	2.25	0.66
1:B:281:ARG:HA	1:B:281:ARG:CZ	2.25	0.66
1:C:211:ASN:ND2	1:D:362:LYS:HD2	2.09	0.66
1:C:510:SER:HA	1:C:521:PRO:HB3	1.78	0.66
1:E:65:GLU:CA	1:E:68:LYS:HE2	2.21	0.66
1:A:251:GLY:HA3	1:A:404:PHE:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:SER:HA	1:B:521:PRO:HB3	1.77	0.66
1:D:266:ASN:HD21	1:D:268:MET:HB2	1.61	0.66
1:E:136:THR:HB	1:E:144:ILE:HD11	1.78	0.66
1:F:224:LEU:HD11	1:F:579:ILE:HD11	1.77	0.66
1:A:319:SER:HA	1:A:322:LEU:HD23	1.78	0.66
1:B:319:SER:HA	1:B:322:LEU:HD23	1.78	0.65
1:D:336:VAL:HG12	1:D:337:GLN:HG2	1.76	0.65
1:C:77:ASP:OD1	1:C:596:ILE:HD13	1.96	0.65
1:F:254:LYS:HD3	1:F:291:GLU:OE1	1.95	0.65
1:B:142:LEU:HD23	1:B:142:LEU:O	1.96	0.65
1:C:381:LYS:O	1:C:385:ARG:HD3	1.96	0.65
1:F:381:LYS:O	1:F:385:ARG:HD3	1.96	0.65
1:C:266:ASN:HD21	1:C:268:MET:HB2	1.61	0.65
1:D:255:ARG:NE	1:D:399:VAL:HG11	2.11	0.65
1:E:255:ARG:NH2	1:E:401:ILE:H	1.94	0.65
1:A:86:ARG:HD2	1:A:201:THR:OG1	1.97	0.65
1:A:457:GLN:HB2	1:A:460:SER:CB	2.26	0.65
1:B:266:ASN:HD21	1:B:268:MET:HB2	1.62	0.65
1:C:319:SER:HA	1:C:322:LEU:HD23	1.79	0.65
1:A:156:PHE:HE1	1:A:229:LEU:HD11	1.62	0.65
1:A:434:VAL:HG13	1:A:548:LEU:HD21	1.78	0.65
1:B:280:LEU:HD12	1:B:384:ILE:HG21	1.78	0.65
1:C:224:LEU:HD11	1:C:579:ILE:HD11	1.78	0.65
1:D:125:LEU:CD1	1:D:148:LEU:HD12	2.26	0.65
1:E:211:ASN:ND2	1:F:362:LYS:HD2	2.12	0.65
1:B:457:GLN:HB2	1:B:460:SER:CB	2.26	0.65
1:F:510:SER:HA	1:F:521:PRO:HB3	1.79	0.65
1:B:122:GLU:N	1:B:122:GLU:OE1	2.30	0.64
1:A:266:ASN:HD21	1:A:268:MET:HB2	1.62	0.64
1:E:132:LEU:HD12	1:E:148:LEU:HD23	1.79	0.64
1:E:179:ARG:O	1:E:183:LEU:HD13	1.96	0.64
1:E:319:SER:HA	1:E:322:LEU:HD23	1.79	0.64
1:F:319:SER:HA	1:F:322:LEU:HD23	1.79	0.64
1:C:443:GLN:HA	1:C:634:ARG:NH2	2.13	0.64
1:C:124:LYS:HG3	1:C:235:ASP:HB3	1.79	0.64
1:E:266:ASN:HD21	1:E:268:MET:HB2	1.62	0.64
1:D:522:LEU:HD13	1:D:526:MET:CE	2.24	0.64
1:E:215:GLY:O	1:E:219:VAL:HG23	1.98	0.64
1:A:135:ALA:O	1:A:139:ARG:HD3	1.98	0.64
1:E:362:LYS:HD2	1:F:211:ASN:ND2	2.12	0.64
1:A:375:LYS:HB2	1:A:375:LYS:HZ2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:VAL:HG12	1:F:296:ILE:HG22	1.78	0.64
1:F:457:GLN:HB2	1:F:460:SER:CB	2.27	0.64
1:F:65:GLU:CA	1:F:68:LYS:HE2	2.21	0.63
1:B:425:ASN:ND2	1:B:428:ASP:H	1.96	0.63
1:C:153:LEU:O	1:C:157:GLN:HG2	1.99	0.63
1:E:472:ARG:HH11	1:E:472:ARG:HG2	1.63	0.63
1:B:122:GLU:HG2	1:B:141:LEU:HD21	1.81	0.63
1:C:457:GLN:HB2	1:C:460:SER:CB	2.26	0.63
1:B:77:ASP:OD1	1:B:596:ILE:HD13	1.99	0.63
1:C:425:ASN:ND2	1:C:428:ASP:H	1.96	0.63
1:D:472:ARG:HH11	1:D:472:ARG:HG2	1.62	0.63
1:F:434:VAL:HG13	1:F:548:LEU:HD21	1.81	0.63
1:F:77:ASP:OD1	1:F:596:ILE:HD13	1.98	0.63
1:A:132:LEU:HD12	1:A:148:LEU:HD22	1.81	0.63
1:B:156:PHE:HE1	1:B:229:LEU:HD11	1.63	0.63
1:B:434:VAL:HG13	1:B:548:LEU:HD21	1.80	0.63
1:C:522:LEU:HD13	1:C:526:MET:CE	2.25	0.63
1:C:434:VAL:HG13	1:C:548:LEU:HD21	1.81	0.63
1:D:285:ILE:HA	1:D:289:ALA:O	1.99	0.63
1:D:457:GLN:HB2	1:D:460:SER:CB	2.28	0.63
1:C:179:ARG:O	1:C:183:LEU:HD13	1.98	0.63
1:C:425:ASN:C	1:C:425:ASN:HD22	2.02	0.63
1:D:510:SER:HA	1:D:521:PRO:HB3	1.79	0.63
1:E:110:SER:HB3	1:E:145:VAL:HG23	1.81	0.63
1:C:375:LYS:HB2	1:C:375:LYS:HZ2	1.63	0.63
1:E:493:THR:HG22	1:E:496:ALA:H	1.63	0.63
1:F:215:GLY:O	1:F:219:VAL:HG23	1.98	0.63
1:B:518:LEU:HD12	1:B:519:GLY:N	2.14	0.63
1:A:522:LEU:HD13	1:A:526:MET:CE	2.28	0.62
1:D:319:SER:HA	1:D:322:LEU:HD23	1.79	0.62
1:A:425:ASN:ND2	1:A:428:ASP:H	1.97	0.62
1:D:156:PHE:HE1	1:D:229:LEU:HD11	1.64	0.62
1:E:544:LEU:HD23	1:E:544:LEU:O	1.99	0.62
1:A:381:LYS:O	1:A:385:ARG:HD3	1.98	0.62
1:A:443:GLN:HA	1:A:634:ARG:NH2	2.13	0.62
1:B:281:ARG:C	1:B:283:GLU:H	2.02	0.62
1:D:125:LEU:HD12	1:D:148:LEU:CD1	2.29	0.62
1:D:77:ASP:OD1	1:D:596:ILE:HD13	1.98	0.62
1:E:509:LEU:CD1	1:E:522:LEU:HB2	2.30	0.62
1:F:606:LYS:HG2	1:F:612:TYR:CD2	2.35	0.62
1:A:102:ILE:HA	1:A:268:MET:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:HD1	1:A:64:GLY:H	1.47	0.62
1:B:443:GLN:HA	1:B:634:ARG:NH2	2.14	0.62
1:E:285:ILE:HA	1:E:289:ALA:O	1.99	0.62
1:B:29:THR:HG23	1:B:31:TRP:N	2.15	0.62
1:E:457:GLN:HB2	1:E:460:SER:CB	2.28	0.62
1:B:63:PHE:HD1	1:B:64:GLY:H	1.48	0.62
1:C:108:HIS:HB2	1:C:114:LEU:HD12	1.80	0.62
1:C:472:ARG:HG2	1:C:472:ARG:NH1	2.15	0.62
1:C:634:ARG:HH11	1:C:634:ARG:HG3	1.64	0.62
1:E:156:PHE:HE1	1:E:229:LEU:HD11	1.64	0.62
1:E:255:ARG:HG2	1:E:401:ILE:HD12	1.82	0.62
1:D:51:ARG:HG2	1:D:57:PRO:HB3	1.80	0.62
1:A:65:GLU:CA	1:A:68:LYS:HE2	2.21	0.62
1:B:117:TYR:CD1	1:B:117:TYR:N	2.67	0.62
1:B:381:LYS:O	1:B:385:ARG:HD3	1.99	0.62
1:E:425:ASN:ND2	1:E:428:ASP:H	1.98	0.62
1:A:425:ASN:HD22	1:A:425:ASN:C	2.03	0.62
1:E:443:GLN:HA	1:E:634:ARG:NH2	2.15	0.62
1:F:336:VAL:HG12	1:F:337:GLN:CG	2.30	0.62
1:B:249:ASN:O	1:B:252:VAL:HG13	1.99	0.61
1:C:51:ARG:HG2	1:C:57:PRO:HB3	1.82	0.61
1:E:425:ASN:HD22	1:E:425:ASN:C	2.02	0.61
1:A:472:ARG:HG2	1:A:472:ARG:NH1	2.14	0.61
1:B:544:LEU:HD23	1:B:544:LEU:O	2.01	0.61
1:B:63:PHE:CZ	1:F:62:PRO:HG3	2.35	0.61
1:F:63:PHE:HD1	1:F:64:GLY:H	1.47	0.61
1:C:156:PHE:HE1	1:C:229:LEU:HD11	1.65	0.61
1:C:509:LEU:CD1	1:C:522:LEU:HB2	2.30	0.61
1:D:103:ALA:HB1	1:D:153:LEU:CD1	2.30	0.61
1:E:381:LYS:O	1:E:385:ARG:HD3	2.00	0.61
1:F:29:THR:HG23	1:F:30:ALA:N	2.15	0.61
1:B:254:LYS:CE	1:B:294:ASN:HB2	2.29	0.61
1:E:103:ALA:HB1	1:E:153:LEU:CD1	2.30	0.61
1:A:137:GLU:OE2	1:A:137:GLU:HA	2.01	0.61
1:A:215:GLY:O	1:A:219:VAL:HG23	2.00	0.61
1:B:103:ALA:HB1	1:B:153:LEU:CD1	2.30	0.61
1:B:51:ARG:HG2	1:B:57:PRO:HB3	1.82	0.61
1:E:51:ARG:HG2	1:E:57:PRO:HB3	1.83	0.61
1:E:434:VAL:HG13	1:E:548:LEU:HD21	1.82	0.61
1:E:362:LYS:HD2	1:F:211:ASN:HD22	1.66	0.61
1:F:522:LEU:HD13	1:F:526:MET:CE	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ILE:HG22	1:D:119:ILE:O	1.99	0.61
1:D:443:GLN:HA	1:D:634:ARG:NH2	2.15	0.61
1:A:29:THR:HG23	1:A:30:ALA:N	2.16	0.61
1:B:110:SER:HB3	1:B:145:VAL:C	2.21	0.61
1:B:119:ILE:HG22	1:B:120:ARG:H	1.59	0.61
1:C:544:LEU:O	1:C:544:LEU:HD23	2.01	0.61
1:D:606:LYS:HG2	1:D:612:TYR:CD2	2.36	0.61
1:E:255:ARG:NH1	1:E:399:VAL:HG12	2.16	0.61
1:E:63:PHE:HD1	1:E:64:GLY:H	1.48	0.61
1:F:124:LYS:HG2	1:F:235:ASP:CB	2.30	0.61
1:F:140:GLY:O	1:F:144:ILE:HD12	2.00	0.61
1:F:425:ASN:C	1:F:425:ASN:HD22	2.03	0.61
1:C:65:GLU:CA	1:C:68:LYS:HE2	2.21	0.61
1:E:202:HIS:HE1	1:F:568:LYS:H	1.49	0.61
1:E:134:VAL:O	1:E:136:THR:HG23	2.00	0.61
1:E:77:ASP:OD1	1:E:596:ILE:HD13	2.00	0.60
1:F:550:VAL:HG22	1:F:554:ASP:OD2	2.01	0.60
1:A:322:LEU:H	1:A:322:LEU:HD22	1.66	0.60
1:B:285:ILE:HA	1:B:289:ALA:O	2.01	0.60
1:D:425:ASN:ND2	1:D:428:ASP:H	1.98	0.60
1:D:65:GLU:CA	1:D:68:LYS:HE2	2.23	0.60
1:E:224:LEU:HD11	1:E:579:ILE:HD11	1.83	0.60
1:C:63:PHE:HD1	1:C:64:GLY:H	1.47	0.60
1:D:29:THR:HG23	1:D:30:ALA:N	2.16	0.60
1:D:381:LYS:O	1:D:385:ARG:HD3	2.01	0.60
1:F:266:ASN:HD21	1:F:268:MET:HB2	1.65	0.60
1:F:51:ARG:HG2	1:F:57:PRO:HB3	1.83	0.60
1:A:544:LEU:HD23	1:A:544:LEU:O	2.01	0.60
1:B:596:ILE:HD12	1:B:596:ILE:H	1.67	0.60
1:D:322:LEU:HD22	1:D:322:LEU:H	1.66	0.60
1:D:215:GLY:O	1:D:219:VAL:HG23	2.02	0.60
1:D:434:VAL:HG13	1:D:548:LEU:HD21	1.84	0.60
1:E:634:ARG:HH11	1:E:634:ARG:HG3	1.67	0.60
1:D:153:LEU:O	1:D:157:GLN:HG2	2.02	0.60
1:C:211:ASN:HD22	1:D:362:LYS:HD2	1.67	0.60
1:E:153:LEU:O	1:E:157:GLN:HG2	2.01	0.60
1:B:127:ALA:HA	1:B:130:LYS:CE	2.31	0.60
1:F:103:ALA:HB1	1:F:153:LEU:CD1	2.31	0.60
1:F:124:LYS:HZ3	1:F:232:GLU:HA	1.67	0.60
1:A:103:ALA:HB1	1:A:153:LEU:CD1	2.30	0.60
1:D:280:LEU:HD23	1:D:280:LEU:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:VAL:HB	1:E:339:ILE:CD1	2.27	0.60
1:D:544:LEU:HD23	1:D:544:LEU:O	2.01	0.60
1:D:63:PHE:HD1	1:D:64:GLY:H	1.50	0.60
1:A:276:VAL:O	1:A:280:LEU:HD13	2.02	0.59
1:F:29:THR:HG23	1:F:31:TRP:N	2.15	0.59
1:A:334:VAL:HB	1:A:339:ILE:CD1	2.26	0.59
1:F:156:PHE:HE1	1:F:229:LEU:HD11	1.66	0.59
1:B:63:PHE:HB2	1:F:46:ALA:HB2	1.84	0.59
1:A:96:SER:HB2	1:A:190:ILE:HG21	1.84	0.59
1:B:336:VAL:HG12	1:B:337:GLN:CG	2.32	0.59
1:B:372:ASP:HB3	1:B:375:LYS:NZ	2.17	0.59
1:B:509:LEU:CD1	1:B:522:LEU:HB2	2.32	0.59
1:C:285:ILE:HA	1:C:289:ALA:O	2.01	0.59
1:E:536:ARG:HG3	1:E:536:ARG:HH11	1.66	0.59
1:F:322:LEU:H	1:F:322:LEU:HD22	1.68	0.59
1:A:596:ILE:H	1:A:596:ILE:HD12	1.67	0.59
1:B:96:SER:HB2	1:B:190:ILE:HG21	1.85	0.59
1:A:205:CYS:SG	1:B:337:GLN:HB3	2.43	0.59
1:D:124:LYS:HE2	1:D:235:ASP:HB2	1.82	0.59
1:F:122:GLU:O	1:F:126:TYR:HD1	1.86	0.59
1:C:103:ALA:HB1	1:C:153:LEU:CD1	2.31	0.59
1:D:375:LYS:HB2	1:D:375:LYS:HZ2	1.68	0.59
1:D:425:ASN:HD22	1:D:425:ASN:C	2.05	0.59
1:A:336:VAL:HG12	1:A:337:GLN:CG	2.31	0.59
1:B:29:THR:HG23	1:B:30:ALA:N	2.17	0.59
1:C:493:THR:HG21	1:C:495:GLU:HG2	1.85	0.59
1:A:372:ASP:HB3	1:A:375:LYS:NZ	2.18	0.59
1:B:322:LEU:HD22	1:B:322:LEU:H	1.67	0.59
1:D:372:ASP:HB3	1:D:375:LYS:NZ	2.18	0.59
1:E:125:LEU:CD2	1:E:145:VAL:HG12	2.33	0.59
1:E:255:ARG:HD3	1:E:399:VAL:CG1	2.28	0.59
1:E:322:LEU:H	1:E:322:LEU:HD22	1.68	0.59
1:E:606:LYS:HG2	1:E:612:TYR:CD2	2.37	0.59
1:F:425:ASN:ND2	1:F:428:ASP:H	2.01	0.59
1:B:215:GLY:O	1:B:219:VAL:HG23	2.02	0.59
1:B:472:ARG:NH1	1:B:472:ARG:HG2	2.17	0.59
1:B:86:ARG:HD2	1:B:201:THR:OG1	2.02	0.59
1:A:139:ARG:HH21	1:A:143:ALA:HB1	1.68	0.59
1:A:606:LYS:HG2	1:A:612:TYR:CD2	2.37	0.59
1:C:501:ALA:HB1	1:C:505:LEU:HD12	1.84	0.59
1:E:29:THR:HG23	1:E:30:ALA:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:ASP:HB3	1:E:375:LYS:NZ	2.16	0.59
1:A:51:ARG:HG2	1:A:57:PRO:HB3	1.85	0.59
1:A:509:LEU:CD1	1:A:522:LEU:HB2	2.32	0.59
1:E:522:LEU:HD13	1:E:526:MET:CE	2.29	0.59
1:A:122:GLU:O	1:A:126:TYR:HB2	2.03	0.58
1:B:280:LEU:HD22	1:B:283:GLU:OE1	2.03	0.58
1:F:285:ILE:HA	1:F:289:ALA:O	2.03	0.58
1:F:493:THR:HG21	1:F:495:GLU:HG2	1.84	0.58
1:A:89:ALA:HB2	1:A:197:THR:HG21	1.84	0.58
1:B:162:ASP:O	1:B:164:PRO:HD3	2.03	0.58
1:D:510:SER:HB3	1:D:521:PRO:HB3	1.86	0.58
1:C:29:THR:HG23	1:C:30:ALA:N	2.18	0.58
1:D:281:ARG:O	1:D:285:ILE:HG13	2.03	0.58
1:F:153:LEU:O	1:F:157:GLN:HG2	2.03	0.58
1:E:501:ALA:HB1	1:E:505:LEU:HD12	1.85	0.58
1:A:29:THR:HG23	1:A:31:TRP:N	2.16	0.58
1:B:89:ALA:HB2	1:B:197:THR:HG21	1.85	0.58
1:A:510:SER:CA	1:A:521:PRO:HB3	2.34	0.58
1:C:334:VAL:HB	1:C:339:ILE:CD1	2.28	0.58
1:F:509:LEU:CD1	1:F:522:LEU:HB2	2.33	0.58
1:A:501:ALA:HB1	1:A:505:LEU:HD12	1.86	0.58
1:D:326:THR:HG22	1:D:328:ALA:H	1.68	0.58
1:E:206:ASP:HB3	1:E:212:LEU:HD21	1.84	0.58
1:E:336:VAL:HG12	1:E:337:GLN:CG	2.34	0.58
1:F:336:VAL:C	1:F:337:GLN:HG2	2.23	0.58
1:A:153:LEU:O	1:A:157:GLN:HG2	2.03	0.58
1:B:550:VAL:HG22	1:B:554:ASP:OD2	2.03	0.58
1:C:536:ARG:HG3	1:C:536:ARG:HH11	1.69	0.58
1:D:86:ARG:HD2	1:D:201:THR:OG1	2.04	0.58
1:D:501:ALA:HB1	1:D:505:LEU:HD12	1.84	0.58
1:B:153:LEU:O	1:B:157:GLN:HG2	2.04	0.57
1:C:550:VAL:HG22	1:C:554:ASP:OD2	2.02	0.57
1:D:509:LEU:CD1	1:D:522:LEU:HB2	2.33	0.57
1:F:536:ARG:HG3	1:F:536:ARG:HH11	1.67	0.57
1:B:280:LEU:HD12	1:B:384:ILE:CG2	2.34	0.57
1:C:606:LYS:HG2	1:C:612:TYR:CD2	2.39	0.57
1:D:29:THR:HG23	1:D:31:TRP:N	2.19	0.57
1:B:117:TYR:HD1	1:B:117:TYR:N	2.02	0.57
1:B:501:ALA:HB1	1:B:505:LEU:HD12	1.86	0.57
1:C:102:ILE:HA	1:C:268:MET:HE2	1.85	0.57
1:D:336:VAL:C	1:D:337:GLN:HG2	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:ARG:HH11	1:D:634:ARG:HG3	1.69	0.57
1:E:102:ILE:HA	1:E:268:MET:HE2	1.86	0.57
1:E:439:ASN:OD1	1:E:441:ASN:ND2	2.36	0.57
1:A:117:TYR:HE1	1:A:373:GLU:HB3	1.69	0.57
1:F:255:ARG:HG3	1:F:401:ILE:HD12	1.85	0.57
1:B:425:ASN:C	1:B:425:ASN:HD22	2.05	0.57
1:D:102:ILE:HA	1:D:268:MET:HE2	1.86	0.57
1:E:89:ALA:HB2	1:E:197:THR:HG21	1.85	0.57
1:A:114:LEU:HD22	1:A:117:TYR:CD1	2.39	0.57
1:A:285:ILE:HA	1:A:289:ALA:O	2.05	0.57
1:E:550:VAL:HG22	1:E:554:ASP:OD2	2.05	0.57
1:F:89:ALA:HB2	1:F:197:THR:HG21	1.85	0.57
1:F:124:LYS:NZ	1:F:232:GLU:HA	2.20	0.57
1:F:472:ARG:NH1	1:F:472:ARG:HG2	2.16	0.57
1:A:122:GLU:CD	1:A:141:LEU:HD22	2.25	0.57
1:B:606:LYS:HG2	1:B:612:TYR:CD2	2.39	0.57
1:C:336:VAL:HG12	1:C:337:GLN:CG	2.35	0.57
1:A:510:SER:HA	1:A:521:PRO:CB	2.34	0.57
1:B:65:GLU:CA	1:B:68:LYS:HE2	2.22	0.57
1:D:253:MET:HE1	1:D:329:LEU:HB2	1.85	0.57
1:C:29:THR:HG23	1:C:31:TRP:N	2.16	0.57
1:D:142:LEU:N	1:D:142:LEU:HD12	2.19	0.57
1:D:266:ASN:ND2	1:D:268:MET:HB2	2.20	0.57
1:E:121:ASP:OD1	1:E:123:ALA:HB3	2.05	0.57
1:A:249:ASN:ND2	1:A:404:PHE:HB2	2.20	0.56
1:B:206:ASP:HB3	1:B:212:LEU:HD21	1.86	0.56
1:A:550:VAL:HG22	1:A:554:ASP:OD2	2.04	0.56
1:B:108:HIS:HB2	1:B:114:LEU:HD12	1.87	0.56
1:B:279:ASP:O	1:B:281:ARG:N	2.38	0.56
1:C:124:LYS:HE2	1:C:235:ASP:HB2	1.86	0.56
1:C:510:SER:HB3	1:C:521:PRO:HB3	1.87	0.56
1:E:249:ASN:HD22	1:E:488:LYS:HE3	1.70	0.56
1:E:211:ASN:HD22	1:F:362:LYS:HD2	1.69	0.56
1:A:510:SER:HB3	1:A:521:PRO:HB3	1.87	0.56
1:C:634:ARG:HG3	1:C:634:ARG:NH1	2.20	0.56
1:A:634:ARG:HH11	1:A:634:ARG:HG3	1.70	0.56
1:B:132:LEU:CD1	1:B:151:ILE:HG21	2.36	0.56
1:C:96:SER:HB2	1:C:190:ILE:HG21	1.87	0.56
1:D:589:PRO:O	1:D:591:VAL:N	2.36	0.56
1:A:493:THR:HG21	1:A:495:GLU:HG2	1.88	0.56
1:E:510:SER:HA	1:E:521:PRO:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:VAL:O	1:C:337:GLN:HG2	2.05	0.56
1:D:206:ASP:HB3	1:D:212:LEU:HD21	1.87	0.56
1:E:96:SER:HB2	1:E:190:ILE:HG21	1.86	0.56
1:F:135:ALA:O	1:F:139:ARG:HD3	2.06	0.56
1:E:336:VAL:C	1:E:337:GLN:HG2	2.25	0.56
1:F:372:ASP:HB3	1:F:375:LYS:NZ	2.20	0.56
1:F:501:ALA:HB1	1:F:505:LEU:HD12	1.88	0.56
1:A:162:ASP:O	1:A:164:PRO:HD3	2.06	0.56
1:B:266:ASN:ND2	1:B:268:MET:HB2	2.21	0.56
1:D:550:VAL:HG22	1:D:554:ASP:OD2	2.06	0.56
1:E:296:ILE:HD12	1:E:314:ALA:HB2	1.88	0.56
1:E:510:SER:HB3	1:E:521:PRO:HB3	1.87	0.56
1:B:536:ARG:HH11	1:B:536:ARG:HG3	1.71	0.56
1:E:472:ARG:NH1	1:E:472:ARG:HG2	2.22	0.56
1:A:439:ASN:OD1	1:A:441:ASN:ND2	2.39	0.55
1:B:281:ARG:NH1	1:B:281:ARG:HA	2.21	0.55
1:B:634:ARG:HH11	1:B:634:ARG:HG3	1.70	0.55
1:D:120:ARG:HG3	1:D:237:LEU:O	2.06	0.55
1:E:189:ASN:HB3	1:E:192:ALA:HB3	1.89	0.55
1:A:118:SER:O	1:A:237:LEU:HD23	2.06	0.55
1:C:266:ASN:ND2	1:C:268:MET:HB2	2.21	0.55
1:F:86:ARG:HD2	1:F:201:THR:OG1	2.06	0.55
1:F:102:ILE:HA	1:F:268:MET:HE2	1.86	0.55
1:F:510:SER:HB3	1:F:521:PRO:HB3	1.86	0.55
1:A:568:LYS:H	1:B:202:HIS:HE1	1.52	0.55
1:C:322:LEU:H	1:C:322:LEU:HD22	1.70	0.55
1:C:510:SER:CA	1:C:521:PRO:HB3	2.37	0.55
1:F:544:LEU:HD23	1:F:544:LEU:O	2.06	0.55
1:A:63:PHE:CG	1:C:46:ALA:HB2	2.42	0.55
1:D:472:ARG:NH1	1:D:472:ARG:HG2	2.20	0.55
1:F:336:VAL:O	1:F:337:GLN:HG2	2.05	0.55
1:F:551:ASP:OD2	1:F:552:LEU:N	2.37	0.55
1:C:568:LYS:H	1:D:202:HIS:HE1	1.54	0.55
1:D:336:VAL:HG12	1:D:337:GLN:CG	2.36	0.55
1:D:536:ARG:HG3	1:D:536:ARG:HH11	1.71	0.55
1:C:372:ASP:HB3	1:C:375:LYS:NZ	2.21	0.55
1:D:63:PHE:CE2	1:E:62:PRO:HG3	2.42	0.55
1:A:536:ARG:HG3	1:A:536:ARG:HH11	1.71	0.55
1:B:334:VAL:HB	1:B:339:ILE:CD1	2.28	0.55
1:B:354:ILE:O	1:B:366:ALA:HB1	2.06	0.55
1:C:362:LYS:HD2	1:D:211:ASN:ND2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:THR:HG21	1:D:495:GLU:HG2	1.89	0.55
1:E:510:SER:CA	1:E:521:PRO:HB3	2.35	0.55
1:B:493:THR:HG21	1:B:495:GLU:HG2	1.87	0.55
1:C:337:GLN:HB3	1:D:205:CYS:SG	2.47	0.55
1:C:550:VAL:HG22	1:C:551:ASP:N	2.21	0.55
1:D:336:VAL:O	1:D:337:GLN:HG2	2.07	0.55
1:E:375:LYS:HZ2	1:E:375:LYS:HB2	1.71	0.55
1:E:86:ARG:HD2	1:E:201:THR:OG1	2.07	0.55
1:C:206:ASP:HB3	1:C:212:LEU:HD21	1.89	0.55
1:C:551:ASP:OD2	1:C:552:LEU:N	2.40	0.55
1:F:125:LEU:HD11	1:F:148:LEU:HD12	1.88	0.55
1:F:252:VAL:HG12	1:F:296:ILE:CG2	2.37	0.55
1:A:206:ASP:HB3	1:A:212:LEU:HD21	1.89	0.54
1:B:462:TYR:CE1	1:B:482:ALA:HA	2.41	0.54
1:C:326:THR:HG22	1:C:328:ALA:H	1.71	0.54
1:D:96:SER:HB2	1:D:190:ILE:HG21	1.88	0.54
1:A:134:VAL:HG21	1:A:148:LEU:HD23	1.88	0.54
1:A:326:THR:HG22	1:A:328:ALA:H	1.72	0.54
1:C:180:LEU:CB	1:C:186:LEU:HD13	2.37	0.54
1:F:296:ILE:HD12	1:F:314:ALA:HB2	1.89	0.54
1:B:510:SER:CA	1:B:521:PRO:HB3	2.37	0.54
1:A:462:TYR:CE1	1:A:482:ALA:HA	2.43	0.54
1:B:336:VAL:C	1:B:337:GLN:HG2	2.28	0.54
1:B:631:GLN:O	1:B:634:ARG:HB2	2.06	0.54
1:E:266:ASN:ND2	1:E:268:MET:HB2	2.21	0.54
1:E:551:ASP:OD2	1:E:552:LEU:N	2.39	0.54
1:F:96:SER:HB2	1:F:190:ILE:HG21	1.89	0.54
1:B:144:ILE:C	1:B:146:GLY:N	2.61	0.54
1:B:510:SER:HB3	1:B:521:PRO:HB3	1.89	0.54
1:C:510:SER:HA	1:C:521:PRO:CB	2.37	0.54
1:E:634:ARG:HG3	1:E:634:ARG:NH1	2.22	0.54
1:F:375:LYS:HZ2	1:F:375:LYS:HB2	1.73	0.54
1:E:162:ASP:O	1:E:164:PRO:HD3	2.08	0.54
1:A:266:ASN:ND2	1:A:268:MET:HB2	2.22	0.54
1:A:296:ILE:HD12	1:A:314:ALA:HB2	1.89	0.54
1:A:336:VAL:C	1:A:337:GLN:HG2	2.26	0.54
1:A:550:VAL:HG22	1:A:551:ASP:N	2.23	0.54
1:B:296:ILE:HD12	1:B:314:ALA:HB2	1.90	0.54
1:C:336:VAL:C	1:C:337:GLN:HG2	2.27	0.54
1:D:510:SER:CA	1:D:521:PRO:HB3	2.38	0.54
1:F:326:THR:HG22	1:F:328:ALA:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:LEU:HD21	1:E:144:ILE:HG22	1.89	0.54
1:C:323:PRO:O	1:C:326:THR:HB	2.08	0.54
1:D:510:SER:HA	1:D:521:PRO:CB	2.38	0.54
1:A:551:ASP:OD2	1:A:552:LEU:N	2.42	0.53
1:B:124:LYS:HE2	1:B:235:ASP:HB3	1.90	0.53
1:B:326:THR:HG22	1:B:328:ALA:H	1.73	0.53
1:B:473:ASN:HA	1:B:505:LEU:HB2	1.90	0.53
1:C:89:ALA:HB2	1:C:197:THR:HG21	1.89	0.53
1:F:462:TYR:CE1	1:F:482:ALA:HA	2.43	0.53
1:F:634:ARG:HH11	1:F:634:ARG:HG3	1.72	0.53
1:E:205:CYS:SG	1:F:337:GLN:HB3	2.47	0.53
1:B:243:PRO:HD3	1:B:416:ALA:HB1	1.90	0.53
1:E:326:THR:HG22	1:E:328:ALA:H	1.73	0.53
1:E:493:THR:HG21	1:E:495:GLU:HG2	1.90	0.53
1:E:589:PRO:O	1:E:591:VAL:N	2.39	0.53
1:D:551:ASP:OD2	1:D:552:LEU:N	2.41	0.53
1:E:550:VAL:HG22	1:E:551:ASP:N	2.22	0.53
1:F:180:LEU:CB	1:F:186:LEU:HD13	2.38	0.53
1:F:206:ASP:HB3	1:F:212:LEU:HD21	1.89	0.53
1:F:335:ASP:CG	1:F:336:VAL:H	2.12	0.53
1:F:493:THR:HG22	1:F:495:GLU:HG2	1.89	0.53
1:B:510:SER:HA	1:B:521:PRO:CB	2.38	0.53
1:D:473:ASN:HA	1:D:505:LEU:HB2	1.91	0.53
1:F:550:VAL:HG22	1:F:551:ASP:N	2.20	0.53
1:A:253:MET:HA	1:A:294:ASN:ND2	2.24	0.53
1:C:296:ILE:HD12	1:C:314:ALA:HB2	1.91	0.53
1:E:29:THR:HG23	1:E:31:TRP:N	2.19	0.53
1:E:336:VAL:O	1:E:337:GLN:HG2	2.09	0.53
1:F:423:LYS:O	1:F:515:ALA:HB1	2.08	0.53
1:E:323:PRO:O	1:E:326:THR:HB	2.08	0.53
1:E:462:TYR:CE1	1:E:482:ALA:HA	2.44	0.53
1:E:596:ILE:H	1:E:596:ILE:HD12	1.72	0.53
1:F:252:VAL:CG1	1:F:296:ILE:HG22	2.39	0.53
1:F:551:ASP:OD2	1:F:552:LEU:HD12	2.09	0.53
1:C:439:ASN:OD1	1:C:441:ASN:ND2	2.42	0.53
1:A:280:LEU:C	1:A:282:ASP:H	2.13	0.53
1:B:281:ARG:O	1:B:283:GLU:N	2.42	0.53
1:B:589:PRO:O	1:B:591:VAL:N	2.40	0.53
1:C:462:TYR:CE1	1:C:482:ALA:HA	2.44	0.53
1:E:254:LYS:HD3	1:E:291:GLU:OE1	2.08	0.53
1:F:510:SER:CA	1:F:521:PRO:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:596:ILE:H	1:F:596:ILE:HD12	1.74	0.53
1:A:110:SER:HB2	1:A:142:LEU:O	2.09	0.53
1:C:335:ASP:CG	1:C:336:VAL:H	2.11	0.53
1:C:69:TYR:O	1:D:37:GLN:NE2	2.41	0.53
1:F:162:ASP:O	1:F:164:PRO:HD3	2.09	0.53
1:C:119:ILE:HG21	1:C:125:LEU:HD22	1.91	0.52
1:C:596:ILE:H	1:C:596:ILE:HD12	1.74	0.52
1:B:335:ASP:CG	1:B:336:VAL:H	2.11	0.52
1:C:141:LEU:C	1:C:143:ALA:H	2.12	0.52
1:D:323:PRO:O	1:D:326:THR:HB	2.09	0.52
1:E:473:ASN:HA	1:E:505:LEU:HB2	1.91	0.52
1:F:189:ASN:HB3	1:F:192:ALA:HB3	1.91	0.52
1:A:493:THR:HG22	1:A:495:GLU:HG2	1.91	0.52
1:F:589:PRO:O	1:F:591:VAL:N	2.42	0.52
1:A:319:SER:CA	1:A:322:LEU:HD23	2.39	0.52
1:B:142:LEU:HA	1:B:145:VAL:CG2	2.39	0.52
1:B:634:ARG:HG3	1:B:634:ARG:NH1	2.25	0.52
1:D:141:LEU:C	1:D:141:LEU:HD13	2.30	0.52
1:F:266:ASN:ND2	1:F:268:MET:HB2	2.23	0.52
1:F:631:GLN:O	1:F:634:ARG:HB2	2.09	0.52
1:D:510:SER:CB	1:D:521:PRO:HB3	2.40	0.52
1:D:631:GLN:O	1:D:634:ARG:HB2	2.10	0.52
1:D:634:ARG:NH1	1:D:634:ARG:HG3	2.24	0.52
1:E:176:ARG:NH2	1:E:609:VAL:O	2.43	0.52
1:F:439:ASN:OD1	1:F:441:ASN:ND2	2.42	0.52
1:A:167:TRP:HZ3	1:A:232:GLU:HG3	1.75	0.52
1:B:141:LEU:C	1:B:143:ALA:H	2.12	0.52
1:B:550:VAL:HG22	1:B:551:ASP:N	2.22	0.52
1:C:473:ASN:HA	1:C:505:LEU:HB2	1.92	0.52
1:C:205:CYS:SG	1:D:337:GLN:HB3	2.49	0.52
1:F:473:ASN:HA	1:F:505:LEU:HB2	1.91	0.52
1:C:86:ARG:HD2	1:C:201:THR:OG1	2.09	0.52
1:E:154:GLY:HA2	1:E:157:GLN:HG3	1.91	0.52
1:A:323:PRO:O	1:A:326:THR:HB	2.10	0.52
1:A:423:LYS:O	1:A:515:ALA:HB1	2.09	0.52
1:A:551:ASP:OD2	1:A:552:LEU:HD12	2.10	0.52
1:A:631:GLN:O	1:A:634:ARG:HB2	2.09	0.52
1:C:140:GLY:O	1:C:144:ILE:HG13	2.10	0.52
1:A:461:ALA:O	1:A:465:LEU:HB2	2.10	0.52
1:B:250:LEU:O	1:B:253:MET:HG3	2.10	0.52
1:B:375:LYS:NZ	1:B:375:LYS:HB2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:PHE:HE2	1:F:62:PRO:CG	2.20	0.52
1:C:103:ALA:HB1	1:C:153:LEU:HD12	1.91	0.52
1:D:124:LYS:HE2	1:D:235:ASP:CB	2.40	0.52
1:D:176:ARG:NH2	1:D:609:VAL:O	2.42	0.52
1:E:493:THR:HG22	1:E:495:GLU:HG2	1.92	0.52
1:A:589:PRO:O	1:A:591:VAL:N	2.42	0.52
1:A:596:ILE:N	1:A:596:ILE:HD12	2.25	0.52
1:B:189:ASN:HB3	1:B:192:ALA:HB3	1.92	0.52
1:B:336:VAL:O	1:B:337:GLN:HG2	2.10	0.52
1:C:493:THR:HG22	1:C:495:GLU:HG2	1.91	0.52
1:D:439:ASN:OD1	1:D:441:ASN:ND2	2.42	0.52
1:D:493:THR:HG22	1:D:495:GLU:HG2	1.90	0.52
1:F:108:HIS:CB	1:F:114:LEU:HD13	2.37	0.52
1:A:197:THR:OG1	1:A:219:VAL:HG21	2.10	0.51
1:B:596:ILE:N	1:B:596:ILE:HD12	2.24	0.51
1:E:335:ASP:CG	1:E:336:VAL:H	2.12	0.51
1:F:510:SER:HA	1:F:521:PRO:CB	2.38	0.51
1:A:510:SER:CB	1:A:521:PRO:HB3	2.40	0.51
1:C:122:GLU:O	1:C:126:TYR:HD1	1.94	0.51
1:C:162:ASP:O	1:C:164:PRO:HD3	2.10	0.51
1:C:589:PRO:O	1:C:591:VAL:N	2.42	0.51
1:D:63:PHE:HE2	1:E:62:PRO:HG3	1.75	0.51
1:F:319:SER:CA	1:F:322:LEU:HD23	2.40	0.51
1:F:250:LEU:CD2	1:F:323:PRO:HG3	2.36	0.51
1:A:156:PHE:CE1	1:A:229:LEU:HD11	2.44	0.51
1:A:63:PHE:CE2	1:C:62:PRO:HG3	2.45	0.51
1:A:63:PHE:HE2	1:C:62:PRO:HG3	1.75	0.51
1:A:202:HIS:CE1	1:B:566:SER:HB2	2.46	0.51
1:B:76:ARG:O	1:B:80:VAL:HG23	2.11	0.51
1:D:132:LEU:HD13	1:D:132:LEU:O	2.10	0.51
1:D:103:ALA:HB1	1:D:153:LEU:HD12	1.91	0.51
1:A:243:PRO:HD3	1:A:416:ALA:HB1	1.92	0.51
1:A:634:ARG:NH1	1:A:634:ARG:HG3	2.25	0.51
1:B:124:LYS:NZ	1:B:235:ASP:HB2	2.26	0.51
1:C:154:GLY:HA2	1:C:157:GLN:HG3	1.92	0.51
1:C:326:THR:HG23	1:C:401:ILE:HG12	1.93	0.51
1:D:462:TYR:CE1	1:D:482:ALA:HA	2.45	0.51
1:D:462:TYR:CE2	1:D:562:PRO:HD2	2.40	0.51
1:E:319:SER:CA	1:E:322:LEU:HD23	2.41	0.51
1:A:103:ALA:HB1	1:A:153:LEU:HD12	1.92	0.51
1:B:375:LYS:HB2	1:B:375:LYS:HZ2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:ASN:ND2	1:C:572:ILE:HD13	2.25	0.51
1:F:29:THR:HG22	1:F:32:HIS:H	1.75	0.51
1:A:330:GLU:HG3	1:A:391:PHE:HA	1.93	0.51
1:C:108:HIS:HB2	1:C:114:LEU:CD1	2.41	0.51
1:D:262:VAL:HG23	1:D:262:VAL:O	2.11	0.51
1:D:296:ILE:HD12	1:D:314:ALA:HB2	1.92	0.51
1:E:281:ARG:O	1:E:285:ILE:HG13	2.11	0.51
1:F:334:VAL:HB	1:F:339:ILE:CD1	2.26	0.51
1:F:48:LEU:HD22	1:F:60:ILE:HB	1.91	0.51
1:A:354:ILE:O	1:A:366:ALA:HB1	2.10	0.51
1:A:375:LYS:HB2	1:A:375:LYS:NZ	2.25	0.51
1:A:473:ASN:HA	1:A:505:LEU:HB2	1.91	0.51
1:B:197:THR:OG1	1:B:219:VAL:HG21	2.10	0.51
1:B:534:ASN:ND2	1:B:572:ILE:HD13	2.26	0.51
1:E:103:ALA:HB1	1:E:153:LEU:HD12	1.91	0.51
1:A:281:ARG:O	1:A:281:ARG:HD2	2.10	0.51
1:B:486:PHE:CD1	1:B:525:VAL:HG11	2.46	0.51
1:C:372:ASP:OD1	1:C:374:HIS:HB2	2.10	0.51
1:D:141:LEU:CD1	1:D:142:LEU:HD12	2.27	0.51
1:F:510:SER:CB	1:F:521:PRO:HB3	2.41	0.51
1:B:176:ARG:NH2	1:B:609:VAL:O	2.44	0.51
1:B:462:TYR:CE2	1:B:562:PRO:HD2	2.40	0.51
1:C:423:LYS:O	1:C:515:ALA:HB1	2.10	0.51
1:F:260:ILE:HB	1:F:295:ILE:HG22	1.93	0.51
1:C:197:THR:OG1	1:C:219:VAL:HG21	2.11	0.50
1:D:121:ASP:OD2	1:D:240:THR:HG22	2.12	0.50
1:D:423:LYS:O	1:D:515:ALA:HB1	2.10	0.50
1:E:243:PRO:HD3	1:E:416:ALA:HB1	1.91	0.50
1:F:317:TYR:O	1:F:320:GLN:HG2	2.10	0.50
1:F:634:ARG:NH1	1:F:634:ARG:HG3	2.26	0.50
1:B:119:ILE:HD12	1:B:119:ILE:N	2.25	0.50
1:B:141:LEU:HA	1:B:144:ILE:CD1	2.38	0.50
1:D:335:ASP:CG	1:D:336:VAL:H	2.14	0.50
1:D:330:GLU:HG3	1:D:391:PHE:HA	1.93	0.50
1:E:447:LEU:HD13	1:E:449:VAL:CG1	2.41	0.50
1:E:510:SER:CB	1:E:521:PRO:HB3	2.40	0.50
1:D:269:LEU:HD13	1:D:371:PHE:CE1	2.46	0.50
1:D:551:ASP:OD2	1:D:552:LEU:HD12	2.11	0.50
1:B:180:LEU:CB	1:B:186:LEU:HD13	2.40	0.50
1:C:105:ALA:HA	1:C:114:LEU:HD11	1.93	0.50
1:C:631:GLN:O	1:C:634:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:SER:CA	1:D:322:LEU:HD23	2.41	0.50
1:A:372:ASP:OD1	1:A:374:HIS:HB2	2.11	0.50
1:C:167:TRP:HB3	1:C:228:MET:HE3	1.93	0.50
1:C:510:SER:CB	1:C:521:PRO:HB3	2.41	0.50
1:D:89:ALA:HB2	1:D:197:THR:HG21	1.92	0.50
1:D:334:VAL:HB	1:D:339:ILE:CD1	2.31	0.50
1:E:156:PHE:CE1	1:E:229:LEU:HD11	2.44	0.50
1:E:257:ALA:HB2	1:E:291:GLU:HB2	1.94	0.50
1:E:631:GLN:O	1:E:634:ARG:HB2	2.11	0.50
1:C:281:ARG:O	1:C:284:ALA:HB3	2.11	0.50
1:C:319:SER:CA	1:C:322:LEU:HD23	2.40	0.50
1:F:372:ASP:OD1	1:F:374:HIS:HB2	2.12	0.50
1:A:126:TYR:CZ	1:A:136:THR:HB	2.47	0.50
1:A:566:SER:HB2	1:B:202:HIS:CE1	2.46	0.50
1:B:384:ILE:O	1:B:388:ILE:HG13	2.10	0.50
1:E:486:PHE:CD1	1:E:525:VAL:HG11	2.46	0.50
1:A:189:ASN:HB3	1:A:192:ALA:HB3	1.94	0.50
1:A:486:PHE:CD1	1:A:525:VAL:HG11	2.47	0.50
1:B:124:LYS:HG3	1:B:240:THR:HG21	1.92	0.50
1:C:354:ILE:O	1:C:366:ALA:HB1	2.12	0.50
1:E:337:GLN:HB3	1:F:205:CYS:SG	2.51	0.50
1:F:326:THR:HG23	1:F:401:ILE:HG12	1.94	0.50
1:A:124:LYS:HD3	1:A:235:ASP:HB3	1.93	0.50
1:D:158:ASN:HD21	1:D:163:LYS:HB3	1.77	0.50
1:A:114:LEU:HD21	1:A:373:GLU:CB	2.42	0.49
1:B:103:ALA:HB1	1:B:153:LEU:HD12	1.92	0.49
1:B:319:SER:CA	1:B:322:LEU:HD23	2.40	0.49
1:D:136:THR:HA	1:D:139:ARG:HG3	1.93	0.49
1:D:534:ASN:ND2	1:D:572:ILE:HD13	2.26	0.49
1:A:326:THR:HG23	1:A:401:ILE:HG12	1.94	0.49
1:A:462:TYR:CE2	1:A:562:PRO:HD2	2.44	0.49
1:A:48:LEU:HD22	1:A:60:ILE:HB	1.93	0.49
1:B:326:THR:HG23	1:B:401:ILE:HG12	1.95	0.49
1:C:250:LEU:CD2	1:C:323:PRO:HG3	2.39	0.49
1:C:551:ASP:OD2	1:C:552:LEU:HD12	2.12	0.49
1:D:550:VAL:HG22	1:D:551:ASP:N	2.23	0.49
1:E:269:LEU:HD13	1:E:371:PHE:CE1	2.47	0.49
1:F:235:ASP:OD1	1:F:240:THR:HA	2.12	0.49
1:F:176:ARG:NH2	1:F:609:VAL:O	2.44	0.49
1:A:518:LEU:O	1:A:520:GLY:N	2.45	0.49
1:B:461:ALA:O	1:B:465:LEU:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:THR:HG22	1:B:495:GLU:HG2	1.91	0.49
1:E:536:ARG:NH1	1:E:536:ARG:HG3	2.27	0.49
1:A:269:LEU:HD13	1:A:371:PHE:CE1	2.48	0.49
1:A:317:TYR:O	1:A:320:GLN:HG2	2.12	0.49
1:A:336:VAL:O	1:A:337:GLN:HG2	2.12	0.49
1:A:337:GLN:HB3	1:B:205:CYS:SG	2.52	0.49
1:B:132:LEU:HD11	1:B:151:ILE:HG21	1.94	0.49
1:B:102:ILE:HA	1:B:268:MET:HE2	1.94	0.49
1:A:37:GLN:NE2	1:B:69:TYR:O	2.43	0.49
1:C:243:PRO:HD3	1:C:416:ALA:HB1	1.94	0.49
1:D:260:ILE:HB	1:D:295:ILE:HG22	1.94	0.49
1:E:235:ASP:OD1	1:E:240:THR:HA	2.13	0.49
1:E:461:ALA:O	1:E:465:LEU:HB2	2.12	0.49
1:F:257:ALA:HB2	1:F:291:GLU:HB2	1.94	0.49
1:F:354:ILE:O	1:F:366:ALA:HB1	2.12	0.49
1:F:62:PRO:HA	1:F:76:ARG:HH22	1.78	0.49
1:A:125:LEU:CD2	1:A:141:LEU:HD11	2.42	0.49
1:D:354:ILE:O	1:D:366:ALA:HB1	2.12	0.49
1:D:447:LEU:HD13	1:D:449:VAL:CG1	2.42	0.49
1:F:154:GLY:HA2	1:F:157:GLN:HG3	1.93	0.49
1:F:326:THR:HG22	1:F:328:ALA:N	2.27	0.49
1:F:518:LEU:CD1	1:F:522:LEU:HD23	2.42	0.49
1:A:154:GLY:HA2	1:A:157:GLN:HG3	1.95	0.49
1:A:192:ALA:O	1:A:196:GLN:HG3	2.12	0.49
1:A:335:ASP:CG	1:A:336:VAL:H	2.15	0.49
1:C:544:LEU:C	1:C:544:LEU:HD23	2.33	0.49
1:D:156:PHE:CE1	1:D:229:LEU:HD11	2.45	0.49
1:E:119:ILE:O	1:E:119:ILE:HG22	2.13	0.49
1:E:85:VAL:CG1	1:E:197:THR:HG23	2.43	0.49
1:F:330:GLU:HG3	1:F:391:PHE:HA	1.95	0.49
1:A:141:LEU:O	1:A:144:ILE:N	2.45	0.49
1:A:69:TYR:O	1:B:37:GLN:NE2	2.40	0.49
1:C:29:THR:HG22	1:C:32:HIS:H	1.77	0.49
1:E:167:TRP:HZ3	1:E:232:GLU:HG3	1.77	0.49
1:F:103:ALA:HB1	1:F:153:LEU:HD12	1.92	0.49
1:A:76:ARG:O	1:A:80:VAL:HG23	2.13	0.49
1:B:122:GLU:O	1:B:125:LEU:N	2.45	0.49
1:B:439:ASN:OD1	1:B:441:ASN:ND2	2.45	0.49
1:B:62:PRO:HG3	1:F:63:PHE:CZ	2.48	0.49
1:C:176:ARG:NH2	1:C:609:VAL:O	2.45	0.49
1:D:137:GLU:O	1:D:138:GLY:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:THR:HG22	1:D:328:ALA:N	2.27	0.49
1:E:372:ASP:OD1	1:E:374:HIS:HB2	2.12	0.49
1:E:330:GLU:HG3	1:E:391:PHE:HA	1.94	0.49
1:F:274:CYS:SG	1:F:295:ILE:HD11	2.53	0.49
1:B:330:GLU:HG3	1:B:391:PHE:HA	1.94	0.49
1:B:423:LYS:O	1:B:515:ALA:HB1	2.12	0.49
1:C:235:ASP:OD1	1:C:240:THR:HA	2.12	0.49
1:C:306:MET:HG2	1:C:410:VAL:HG21	1.95	0.49
1:D:162:ASP:O	1:D:164:PRO:HD3	2.12	0.49
1:D:306:MET:HG2	1:D:410:VAL:HG21	1.94	0.49
1:B:167:TRP:HZ3	1:B:232:GLU:HG3	1.78	0.49
1:B:269:LEU:HD13	1:B:371:PHE:CE1	2.48	0.49
1:B:48:LEU:HD22	1:B:60:ILE:HB	1.93	0.49
1:D:486:PHE:CD1	1:D:525:VAL:HG11	2.48	0.49
1:D:498:THR:HA	1:D:506:LYS:HE2	1.94	0.49
1:E:132:LEU:HD12	1:E:148:LEU:HD22	1.94	0.49
1:B:323:PRO:O	1:B:326:THR:HB	2.12	0.48
1:D:154:GLY:HA2	1:D:157:GLN:HG3	1.94	0.48
1:D:596:ILE:H	1:D:596:ILE:HD12	1.77	0.48
1:F:534:ASN:ND2	1:F:572:ILE:HD13	2.28	0.48
1:B:276:VAL:O	1:B:280:LEU:HG	2.13	0.48
1:C:282:ASP:O	1:C:284:ALA:N	2.46	0.48
1:C:428:ASP:O	1:C:431:LYS:HB3	2.13	0.48
1:C:486:PHE:CD1	1:C:525:VAL:HG11	2.48	0.48
1:D:251:GLY:CA	1:D:404:PHE:O	2.60	0.48
1:E:534:ASN:ND2	1:E:572:ILE:HD13	2.29	0.48
1:F:536:ARG:HG3	1:F:536:ARG:NH1	2.28	0.48
1:A:157:GLN:HB3	1:B:157:GLN:HB3	1.95	0.48
1:B:317:TYR:O	1:B:320:GLN:HG2	2.13	0.48
1:D:136:THR:O	1:D:139:ARG:HB2	2.13	0.48
1:D:372:ASP:OD1	1:D:374:HIS:HB2	2.12	0.48
1:D:375:LYS:HB2	1:D:375:LYS:NZ	2.27	0.48
1:E:423:LYS:O	1:E:515:ALA:HB1	2.13	0.48
1:E:596:ILE:N	1:E:596:ILE:HD12	2.28	0.48
1:F:243:PRO:HD3	1:F:416:ALA:HB1	1.93	0.48
1:B:118:SER:C	1:B:119:ILE:HD12	2.33	0.48
1:A:517:GLY:C	1:A:518:LEU:HD13	2.33	0.48
1:B:122:GLU:C	1:B:124:LYS:N	2.65	0.48
1:B:132:LEU:C	1:B:134:VAL:H	2.17	0.48
1:C:122:GLU:OE1	1:C:141:LEU:HD22	2.13	0.48
1:C:375:LYS:HB2	1:C:375:LYS:NZ	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:TRP:HZ3	1:D:232:GLU:HG3	1.77	0.48
1:E:252:VAL:HG12	1:E:296:ILE:HG22	1.95	0.48
1:F:462:TYR:CE2	1:F:562:PRO:HD2	2.41	0.48
1:B:130:LYS:C	1:B:132:LEU:H	2.16	0.48
1:B:260:ILE:HB	1:B:295:ILE:HG22	1.96	0.48
1:B:510:SER:CB	1:B:521:PRO:HB3	2.43	0.48
1:B:551:ASP:OD2	1:B:552:LEU:N	2.44	0.48
1:C:317:TYR:O	1:C:320:GLN:HG2	2.13	0.48
1:D:85:VAL:HG12	1:D:197:THR:CG2	2.44	0.48
1:E:134:VAL:HG22	1:E:134:VAL:O	2.13	0.48
1:E:274:CYS:SG	1:E:295:ILE:HD11	2.54	0.48
1:E:544:LEU:C	1:E:544:LEU:HD23	2.33	0.48
1:B:544:LEU:C	1:B:544:LEU:HD23	2.33	0.48
1:B:95:HIS:O	1:B:98:HIS:HB3	2.13	0.48
1:C:224:LEU:HD22	1:C:228:MET:HG3	1.96	0.48
1:D:257:ALA:HB2	1:D:291:GLU:HB2	1.95	0.48
1:F:486:PHE:CD1	1:F:525:VAL:HG11	2.48	0.48
1:B:372:ASP:OD1	1:B:374:HIS:HB2	2.13	0.48
1:D:132:LEU:CD1	1:D:151:ILE:HD13	2.43	0.48
1:D:61:ASP:O	1:D:68:LYS:NZ	2.46	0.48
1:F:167:TRP:HZ3	1:F:232:GLU:HG3	1.78	0.48
1:F:493:THR:HG23	1:F:495:GLU:OE2	2.13	0.48
1:A:129:ALA:HA	1:A:148:LEU:HD21	1.96	0.48
1:C:167:TRP:HZ3	1:C:232:GLU:HG3	1.78	0.48
1:C:71:VAL:O	1:C:71:VAL:HG12	2.14	0.48
1:C:330:GLU:HG3	1:C:391:PHE:HA	1.96	0.47
1:E:310:GLY:O	1:E:311:VAL:C	2.52	0.47
1:F:323:PRO:O	1:F:326:THR:HB	2.13	0.47
1:A:280:LEU:C	1:A:282:ASP:N	2.67	0.47
1:B:260:ILE:O	1:B:295:ILE:HA	2.14	0.47
1:B:29:THR:HG22	1:B:32:HIS:H	1.78	0.47
1:B:428:ASP:O	1:B:431:LYS:HB3	2.13	0.47
1:C:462:TYR:CE2	1:C:562:PRO:HD2	2.45	0.47
1:D:358:ASP:OD1	1:D:360:HIS:N	2.42	0.47
1:F:428:ASP:O	1:F:431:LYS:HB3	2.14	0.47
1:A:251:GLY:O	1:A:405:LYS:HG3	2.13	0.47
1:A:326:THR:HG22	1:A:328:ALA:N	2.29	0.47
1:A:534:ASN:ND2	1:A:572:ILE:HD13	2.29	0.47
1:B:154:GLY:HA2	1:B:157:GLN:HG3	1.96	0.47
1:D:310:GLY:O	1:D:311:VAL:C	2.53	0.47
1:D:384:ILE:O	1:D:388:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:PRO:HD3	1:D:416:ALA:HB1	1.95	0.47
1:E:180:LEU:CB	1:E:186:LEU:HD13	2.44	0.47
1:E:260:ILE:HB	1:E:295:ILE:HG22	1.96	0.47
1:E:326:THR:HG22	1:E:328:ALA:N	2.29	0.47
1:E:69:TYR:O	1:F:37:GLN:NE2	2.45	0.47
1:A:544:LEU:HD23	1:A:544:LEU:C	2.34	0.47
1:B:187:PRO:HD3	1:B:221:MET:HB2	1.96	0.47
1:B:80:VAL:HG13	1:B:590:PRO:O	2.15	0.47
1:C:156:PHE:CE1	1:C:229:LEU:HD11	2.47	0.47
1:C:326:THR:HG22	1:C:328:ALA:N	2.29	0.47
1:D:461:ALA:O	1:D:465:LEU:HB2	2.14	0.47
1:E:498:THR:HA	1:E:506:LYS:HE2	1.97	0.47
1:A:257:ALA:HB2	1:A:291:GLU:HB2	1.96	0.47
1:B:326:THR:HG22	1:B:328:ALA:N	2.29	0.47
1:B:61:ASP:O	1:B:68:LYS:NZ	2.48	0.47
1:C:358:ASP:OD1	1:C:360:HIS:N	2.42	0.47
1:E:129:ALA:HB1	1:E:134:VAL:HG13	1.96	0.47
1:E:132:LEU:HD13	1:E:151:ILE:HG21	1.95	0.47
1:E:262:VAL:O	1:E:262:VAL:HG23	2.14	0.47
1:E:354:ILE:O	1:E:366:ALA:HB1	2.13	0.47
1:A:306:MET:HG2	1:A:410:VAL:HG21	1.97	0.47
1:B:358:ASP:OD1	1:B:360:HIS:N	2.40	0.47
1:B:551:ASP:OD2	1:B:552:LEU:HD12	2.14	0.47
1:C:257:ALA:HB2	1:C:291:GLU:HB2	1.96	0.47
1:D:29:THR:HG22	1:D:32:HIS:H	1.78	0.47
1:D:46:ALA:HB2	1:E:63:PHE:CG	2.49	0.47
1:E:125:LEU:HD22	1:E:145:VAL:HG12	1.96	0.47
1:E:250:LEU:HD23	1:E:250:LEU:N	2.29	0.47
1:D:62:PRO:HG3	1:E:63:PHE:CE2	2.49	0.47
1:F:498:THR:HA	1:F:506:LYS:HE2	1.97	0.47
1:F:517:GLY:C	1:F:519:GLY:H	2.18	0.47
1:A:126:TYR:CE2	1:A:136:THR:CB	2.96	0.47
1:A:384:ILE:O	1:A:388:ILE:HG13	2.14	0.47
1:A:61:ASP:O	1:A:68:LYS:NZ	2.47	0.47
1:B:235:ASP:OD1	1:B:240:THR:HA	2.15	0.47
1:B:561:ALA:HB1	1:B:564:CYS:HB3	1.97	0.47
1:C:125:LEU:HD11	1:C:148:LEU:HD12	1.97	0.47
1:A:63:PHE:HB2	1:C:46:ALA:HB2	1.96	0.47
1:E:375:LYS:HB2	1:E:375:LYS:NZ	2.29	0.47
1:E:326:THR:HG23	1:E:401:ILE:HG12	1.96	0.47
1:F:187:PRO:HD3	1:F:221:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:461:ALA:O	1:F:465:LEU:HB2	2.15	0.47
1:A:161:TYR:OH	1:B:360:HIS:HE1	1.97	0.47
1:A:391:PHE:O	1:A:394:ARG:HB3	2.15	0.47
1:B:128:ILE:HA	1:B:131:THR:HB	1.95	0.47
1:B:192:ALA:O	1:B:196:GLN:HG3	2.14	0.47
1:B:62:PRO:HA	1:B:76:ARG:HH22	1.80	0.47
1:C:391:PHE:O	1:C:394:ARG:HB3	2.14	0.47
1:C:461:ALA:O	1:C:465:LEU:HB2	2.14	0.47
1:C:493:THR:HG23	1:C:495:GLU:OE2	2.14	0.47
1:C:498:THR:HA	1:C:506:LYS:HE2	1.96	0.47
1:D:544:LEU:C	1:D:544:LEU:HD23	2.35	0.47
1:E:251:GLY:HA3	1:E:404:PHE:O	2.15	0.47
1:E:261:ALA:HA	1:E:296:ILE:O	2.14	0.47
1:F:262:VAL:O	1:F:262:VAL:HG23	2.13	0.47
1:A:260:ILE:HB	1:A:295:ILE:HG22	1.96	0.47
1:B:257:ALA:HB2	1:B:291:GLU:HB2	1.96	0.47
1:D:167:TRP:HB3	1:D:228:MET:HE3	1.95	0.47
1:D:251:GLY:O	1:D:405:LYS:HB2	2.15	0.47
1:E:29:THR:HG22	1:E:32:HIS:H	1.79	0.47
1:F:261:ALA:HA	1:F:296:ILE:O	2.15	0.47
1:F:375:LYS:NZ	1:F:375:LYS:HB2	2.29	0.47
1:A:283:GLU:O	1:A:286:ALA:HB3	2.14	0.47
1:C:105:ALA:HA	1:C:114:LEU:CD1	2.45	0.47
1:C:536:ARG:NH1	1:C:536:ARG:HG3	2.28	0.47
1:D:197:THR:OG1	1:D:219:VAL:HG21	2.15	0.47
1:E:61:ASP:O	1:E:68:LYS:NZ	2.48	0.47
1:F:105:ALA:O	1:F:109:ILE:HG13	2.14	0.47
1:A:29:THR:HG22	1:A:32:HIS:H	1.79	0.47
1:B:501:ALA:O	1:B:506:LYS:HE3	2.15	0.47
1:C:260:ILE:HB	1:C:295:ILE:HG22	1.97	0.47
1:D:536:ARG:NH1	1:D:536:ARG:HG3	2.30	0.47
1:E:428:ASP:O	1:E:431:LYS:HB3	2.14	0.47
1:F:255:ARG:HG2	1:F:399:VAL:HG11	1.97	0.47
1:A:276:VAL:HG21	1:A:380:ALA:HB3	1.97	0.46
1:A:425:ASN:HD22	1:A:427:ASP:H	1.63	0.46
1:A:428:ASP:O	1:A:431:LYS:HB3	2.14	0.46
1:A:498:THR:HA	1:A:506:LYS:HE2	1.97	0.46
1:B:306:MET:HG2	1:B:410:VAL:HG21	1.97	0.46
1:B:391:PHE:O	1:B:394:ARG:HB3	2.14	0.46
1:D:279:ASP:C	1:D:280:LEU:HD23	2.35	0.46
1:D:327:GLY:O	1:D:394:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:ALA:HB1	1:D:564:CYS:HB3	1.95	0.46
1:E:551:ASP:OD2	1:E:552:LEU:HD12	2.15	0.46
1:F:76:ARG:O	1:F:80:VAL:HG23	2.15	0.46
1:A:261:ALA:HA	1:A:296:ILE:O	2.16	0.46
1:C:105:ALA:O	1:C:109:ILE:HG13	2.14	0.46
1:C:122:GLU:OE1	1:C:141:LEU:CD2	2.64	0.46
1:C:280:LEU:O	1:C:281:ARG:C	2.53	0.46
1:E:116:ASP:OD2	1:E:116:ASP:N	2.48	0.46
1:B:158:ASN:HD21	1:B:163:LYS:HB3	1.80	0.46
1:B:262:VAL:HG23	1:B:262:VAL:O	2.15	0.46
1:A:345:ARG:NH2	1:B:73:GLY:O	2.48	0.46
1:C:189:ASN:HB3	1:C:192:ALA:HB3	1.97	0.46
1:D:189:ASN:HB3	1:D:192:ALA:HB3	1.97	0.46
1:D:95:HIS:O	1:D:98:HIS:HB3	2.16	0.46
1:E:31:TRP:HZ3	1:E:322:LEU:HD21	1.79	0.46
1:E:462:TYR:CE2	1:E:562:PRO:HD2	2.43	0.46
1:F:147:ASP:O	1:F:151:ILE:HG13	2.16	0.46
1:F:156:PHE:CE1	1:F:229:LEU:HD11	2.47	0.46
1:F:384:ILE:O	1:F:388:ILE:HG13	2.15	0.46
1:F:61:ASP:O	1:F:68:LYS:NZ	2.48	0.46
1:A:167:TRP:HB3	1:A:228:MET:HE3	1.98	0.46
1:B:536:ARG:NH1	1:B:536:ARG:HG3	2.30	0.46
1:C:425:ASN:HD22	1:C:427:ASP:H	1.64	0.46
1:D:317:TYR:O	1:D:320:GLN:HG2	2.15	0.46
1:D:428:ASP:O	1:D:431:LYS:HB3	2.15	0.46
1:E:167:TRP:HB3	1:E:228:MET:HE3	1.97	0.46
1:D:63:PHE:CG	1:E:46:ALA:HB2	2.50	0.46
1:F:110:SER:HB2	1:F:142:LEU:O	2.16	0.46
1:F:306:MET:HG2	1:F:410:VAL:HG21	1.96	0.46
1:F:391:PHE:O	1:F:394:ARG:HB3	2.16	0.46
1:F:596:ILE:N	1:F:596:ILE:HD12	2.30	0.46
1:C:48:LEU:HD22	1:C:60:ILE:HB	1.97	0.46
1:D:180:LEU:CB	1:D:186:LEU:HD13	2.42	0.46
1:D:85:VAL:CG1	1:D:197:THR:HG23	2.45	0.46
1:D:493:THR:HG23	1:D:495:GLU:OE2	2.15	0.46
1:E:85:VAL:HG12	1:E:197:THR:CG2	2.45	0.46
1:B:122:GLU:C	1:B:124:LYS:H	2.19	0.46
1:B:276:VAL:HG21	1:B:380:ALA:HB3	1.98	0.46
1:C:80:VAL:HG13	1:C:590:PRO:O	2.16	0.46
1:D:126:TYR:O	1:D:129:ALA:HB3	2.15	0.46
1:E:358:ASP:OD1	1:E:360:HIS:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:LEU:HD13	1:F:371:PHE:CE1	2.51	0.46
1:B:193:SER:HB3	1:B:219:VAL:HG13	1.98	0.46
1:B:261:ALA:HA	1:B:296:ILE:O	2.15	0.46
1:C:62:PRO:HA	1:C:76:ARG:HH22	1.80	0.46
1:F:459:ASP:HB3	1:F:485:ALA:HB1	1.97	0.46
1:B:109:ILE:CD1	1:B:237:LEU:HD21	2.46	0.46
1:C:158:ASN:HD21	1:C:163:LYS:HB3	1.80	0.46
1:C:31:TRP:HZ3	1:C:322:LEU:HD21	1.80	0.46
1:C:362:LYS:HD2	1:D:211:ASN:HD22	1.81	0.46
1:A:62:PRO:HA	1:A:76:ARG:HH22	1.80	0.46
1:F:185:LEU:HD21	1:F:214:LEU:HD22	1.97	0.46
1:F:310:GLY:O	1:F:311:VAL:C	2.54	0.46
1:A:536:ARG:HG3	1:A:536:ARG:NH1	2.29	0.46
1:A:450:GLY:O	4:A:800:WCC:S1	2.74	0.46
1:B:450:GLY:O	4:B:800:WCC:S1	2.74	0.46
1:C:596:ILE:N	1:C:596:ILE:HD12	2.30	0.46
1:D:552:LEU:HD12	1:D:552:LEU:H	1.81	0.46
1:F:29:THR:HG21	1:F:31:TRP:HE3	1.81	0.46
1:C:261:ALA:HA	1:C:296:ILE:O	2.15	0.45
1:D:132:LEU:HD12	1:D:151:ILE:HD12	1.99	0.45
1:D:250:LEU:CD1	1:D:323:PRO:HG3	2.46	0.45
1:C:457:GLN:O	1:C:458:GLN:C	2.55	0.45
1:D:261:ALA:HA	1:D:296:ILE:O	2.15	0.45
1:D:31:TRP:HZ3	1:D:322:LEU:HD21	1.81	0.45
1:E:307:MET:HG3	1:E:529:GLY:HA2	1.99	0.45
1:E:124:LYS:NZ	1:E:415:GLU:OE2	2.49	0.45
1:E:561:ALA:HB1	1:E:564:CYS:HB3	1.98	0.45
1:D:176:ARG:NH1	1:D:551:ASP:OD1	2.50	0.45
1:F:457:GLN:O	1:F:458:GLN:C	2.54	0.45
1:F:544:LEU:HD23	1:F:544:LEU:C	2.36	0.45
1:A:85:VAL:CG1	1:A:197:THR:HG23	2.46	0.45
1:B:127:ALA:HA	1:B:130:LYS:HG2	1.98	0.45
1:B:31:TRP:HZ3	1:B:322:LEU:HD21	1.81	0.45
1:C:142:LEU:HD23	1:C:142:LEU:N	2.32	0.45
1:C:204:GLY:O	1:D:337:GLN:HA	2.16	0.45
1:E:224:LEU:O	1:E:228:MET:HG3	2.17	0.45
1:E:306:MET:HG2	1:E:410:VAL:HG21	1.97	0.45
1:E:48:LEU:HD22	1:E:60:ILE:HB	1.99	0.45
1:A:280:LEU:HD23	1:A:388:ILE:HD11	1.97	0.45
1:A:561:ALA:HB1	1:A:564:CYS:HB3	1.98	0.45
1:A:80:VAL:HG13	1:A:590:PRO:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLU:O	1:B:114:LEU:HB2	2.16	0.45
1:B:116:ASP:HB2	1:B:117:TYR:CD1	2.52	0.45
1:B:129:ALA:HA	1:B:134:VAL:HG21	1.99	0.45
1:C:424:VAL:HG13	1:C:432:PRO:HG3	1.98	0.45
1:D:48:LEU:HD22	1:D:60:ILE:HB	1.97	0.45
1:E:254:LYS:HB2	1:E:257:ALA:HB3	1.97	0.45
1:A:180:LEU:CB	1:A:186:LEU:HD13	2.41	0.45
1:B:124:LYS:O	1:B:127:ALA:HB3	2.16	0.45
1:C:124:LYS:HE2	1:C:235:ASP:CB	2.46	0.45
1:E:110:SER:HB3	1:E:145:VAL:HG22	1.97	0.45
1:E:317:TYR:O	1:E:320:GLN:HG2	2.16	0.45
1:F:254:LYS:HB2	1:F:257:ALA:HB3	1.97	0.45
1:A:114:LEU:HD21	1:A:373:GLU:C	2.37	0.45
1:A:260:ILE:O	1:A:295:ILE:HA	2.17	0.45
1:A:31:TRP:HZ3	1:A:322:LEU:HD21	1.81	0.45
1:A:493:THR:HG23	1:A:495:GLU:OE2	2.16	0.45
1:B:38:GLN:HA	1:B:38:GLN:OE1	2.17	0.45
1:C:337:GLN:HB3	1:C:337:GLN:HE21	1.62	0.45
1:C:384:ILE:O	1:C:388:ILE:HG13	2.17	0.45
1:C:61:ASP:O	1:C:68:LYS:NZ	2.49	0.45
1:D:38:GLN:OE1	1:D:40:GLN:HG3	2.17	0.45
1:E:384:ILE:O	1:E:388:ILE:HG13	2.17	0.45
1:E:255:ARG:CZ	1:E:399:VAL:HG12	2.47	0.45
1:F:424:VAL:O	1:F:425:ASN:HB2	2.16	0.45
1:A:167:TRP:CZ3	1:A:232:GLU:HG3	2.52	0.45
1:C:262:VAL:HG23	1:C:262:VAL:O	2.17	0.45
1:C:447:LEU:HD13	1:C:449:VAL:CG1	2.47	0.45
1:D:263:ASN:HB2	1:D:298:ILE:HB	1.98	0.45
1:E:37:GLN:NE2	1:F:69:TYR:O	2.44	0.45
1:A:38:GLN:HA	1:A:38:GLN:OE1	2.17	0.45
1:A:95:HIS:O	1:A:98:HIS:HB3	2.16	0.45
1:B:156:PHE:CE1	1:B:229:LEU:HD11	2.46	0.45
1:C:459:ASP:HB3	1:C:485:ALA:HB1	1.99	0.45
1:C:450:GLY:O	4:C:800:WCC:S1	2.75	0.45
1:D:235:ASP:OD1	1:D:240:THR:HA	2.16	0.45
1:D:269:LEU:HD13	1:D:371:PHE:CD1	2.52	0.45
1:D:596:ILE:N	1:D:596:ILE:HD12	2.32	0.45
1:E:250:LEU:C	1:E:252:VAL:H	2.20	0.45
1:E:499:GLN:O	1:E:499:GLN:HG2	2.17	0.45
1:A:251:GLY:O	1:A:405:LYS:HB2	2.17	0.45
1:B:167:TRP:HB3	1:B:228:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:C	1:B:283:GLU:N	2.67	0.45
1:C:109:ILE:CD1	1:C:237:LEU:HD21	2.47	0.45
1:C:269:LEU:HD13	1:C:371:PHE:CE1	2.52	0.45
1:D:425:ASN:HD22	1:D:427:ASP:H	1.65	0.45
1:E:125:LEU:CD2	1:E:144:ILE:HG22	2.45	0.45
1:E:279:ASP:C	1:E:281:ARG:H	2.20	0.45
1:E:319:SER:O	1:E:323:PRO:HD3	2.17	0.45
1:F:471:LYS:C	1:F:473:ASN:H	2.20	0.45
1:A:281:ARG:C	1:A:281:ARG:HD2	2.38	0.44
1:A:310:GLY:O	1:A:311:VAL:C	2.55	0.44
1:B:309:HIS:N	1:B:309:HIS:ND1	2.65	0.44
1:C:319:SER:HA	1:C:322:LEU:CD2	2.46	0.44
1:E:197:THR:OG1	1:E:219:VAL:HG21	2.18	0.44
1:E:326:THR:CG2	1:E:328:ALA:HB3	2.47	0.44
1:E:269:LEU:HD13	1:E:371:PHE:CD1	2.52	0.44
1:E:424:VAL:HG13	1:E:432:PRO:HG3	1.98	0.44
1:C:149:ALA:O	1:C:153:LEU:HB2	2.16	0.44
1:E:144:ILE:C	1:E:146:GLY:H	2.20	0.44
1:E:193:SER:HB3	1:E:219:VAL:HG13	1.99	0.44
1:E:276:VAL:HG21	1:E:380:ALA:HB3	1.99	0.44
1:F:194:VAL:O	1:F:197:THR:HB	2.18	0.44
1:F:319:SER:HA	1:F:322:LEU:CD2	2.46	0.44
1:A:211:ASN:ND2	1:B:362:LYS:CD	2.73	0.44
1:A:87:MET:O	1:A:567:GLU:HB3	2.18	0.44
1:B:250:LEU:HD21	1:B:323:PRO:CG	2.40	0.44
1:D:119:ILE:HG22	1:D:122:GLU:HG2	2.00	0.44
1:D:337:GLN:HB3	1:D:337:GLN:HE21	1.61	0.44
1:F:424:VAL:HG13	1:F:432:PRO:HG3	1.99	0.44
1:A:202:HIS:HB3	1:A:205:CYS:SG	2.57	0.44
1:B:130:LYS:HD2	1:B:131:THR:N	2.33	0.44
1:B:278:ALA:O	1:B:281:ARG:HG2	2.17	0.44
1:B:310:GLY:O	1:B:311:VAL:C	2.55	0.44
1:B:493:THR:HG23	1:B:495:GLU:OE2	2.16	0.44
1:C:282:ASP:O	1:C:283:GLU:C	2.55	0.44
1:C:532:VAL:C	1:C:534:ASN:H	2.21	0.44
1:E:425:ASN:HD22	1:E:427:ASP:H	1.65	0.44
1:F:117:TYR:CD1	1:F:117:TYR:N	2.85	0.44
1:F:192:ALA:O	1:F:196:GLN:HG3	2.17	0.44
1:F:31:TRP:HZ3	1:F:322:LEU:HD21	1.82	0.44
1:F:85:VAL:HG12	1:F:197:THR:CG2	2.48	0.44
1:A:319:SER:HA	1:A:322:LEU:CD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:O	1:B:345:ARG:NH2	2.51	0.44
1:A:85:VAL:HG12	1:A:197:THR:CG2	2.47	0.44
1:B:29:THR:HG21	1:B:31:TRP:HE3	1.82	0.44
1:C:185:LEU:HD21	1:C:214:LEU:HD22	1.99	0.44
1:C:193:SER:HB3	1:C:219:VAL:HG13	1.99	0.44
1:C:263:ASN:HB2	1:C:298:ILE:HB	1.99	0.44
1:C:515:ALA:C	1:C:517:GLY:H	2.21	0.44
1:D:326:THR:HG23	1:D:401:ILE:HG12	1.98	0.44
1:E:202:HIS:HB3	1:E:205:CYS:SG	2.58	0.44
1:E:109:ILE:CD1	1:E:237:LEU:HD21	2.48	0.44
1:F:260:ILE:O	1:F:295:ILE:HA	2.18	0.44
1:F:552:LEU:H	1:F:552:LEU:HD12	1.82	0.44
1:A:96:SER:CB	1:A:190:ILE:HG21	2.47	0.44
1:B:185:LEU:HD21	1:B:214:LEU:HD22	2.00	0.44
1:C:274:CYS:SG	1:C:295:ILE:HD11	2.58	0.44
1:D:158:ASN:ND2	1:D:163:LYS:HE3	2.31	0.44
1:E:144:ILE:C	1:E:146:GLY:N	2.70	0.44
1:F:193:SER:HB3	1:F:219:VAL:HG13	1.98	0.44
1:F:276:VAL:HG21	1:F:380:ALA:HB3	2.00	0.44
1:F:38:GLN:OE1	1:F:40:GLN:HG3	2.18	0.44
1:A:326:THR:CG2	1:A:328:ALA:HB3	2.48	0.44
1:A:33:ARG:NH1	1:B:71:VAL:O	2.50	0.44
1:A:269:LEU:HD13	1:A:371:PHE:CD1	2.53	0.44
1:A:514:THR:C	1:A:516:ALA:N	2.71	0.44
1:B:229:LEU:C	1:B:229:LEU:HD23	2.38	0.44
1:B:85:VAL:CG1	1:B:197:THR:HG23	2.48	0.44
1:C:560:SER:C	1:C:562:PRO:HD3	2.38	0.44
1:E:327:GLY:O	1:E:394:ARG:HD3	2.17	0.44
1:E:457:GLN:O	1:E:458:GLN:C	2.56	0.44
1:A:109:ILE:CD1	1:A:237:LEU:HD21	2.48	0.44
1:A:125:LEU:HD21	1:A:141:LEU:HD11	1.99	0.44
1:A:235:ASP:OD1	1:A:240:THR:HA	2.17	0.44
1:A:249:ASN:O	1:A:252:VAL:HG22	2.18	0.44
1:A:421:LEU:HB3	1:A:429:PRO:O	2.17	0.44
1:B:327:GLY:O	1:B:394:ARG:HD3	2.17	0.44
1:C:316:ASN:HB2	1:C:317:TYR:H	1.62	0.44
1:C:499:GLN:HG2	1:C:499:GLN:O	2.18	0.44
1:D:276:VAL:HG21	1:D:380:ALA:HB3	2.00	0.44
1:F:425:ASN:HD22	1:F:427:ASP:H	1.65	0.44
1:F:85:VAL:CG1	1:F:197:THR:HG23	2.48	0.44
1:A:187:PRO:HD3	1:A:221:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LEU:C	1:C:229:LEU:HD23	2.38	0.44
1:C:29:THR:HG21	1:C:31:TRP:HE3	1.82	0.44
1:C:561:ALA:HB1	1:C:564:CYS:HB3	2.00	0.44
1:D:132:LEU:CD1	1:D:151:ILE:CD1	2.95	0.44
1:D:391:PHE:O	1:D:394:ARG:HB3	2.17	0.44
1:E:62:PRO:HA	1:E:76:ARG:HH22	1.81	0.44
1:F:152:THR:HG23	1:F:229:LEU:HG	1.99	0.44
1:F:502:GLY:O	1:F:503:GLU:C	2.56	0.44
1:A:457:GLN:O	1:A:458:GLN:C	2.56	0.43
1:A:62:PRO:HA	1:A:76:ARG:NH2	2.33	0.43
1:B:102:ILE:HG12	1:B:268:MET:HE2	2.00	0.43
1:B:144:ILE:HG12	1:B:144:ILE:H	1.42	0.43
1:B:274:CYS:SG	1:B:295:ILE:HD11	2.58	0.43
1:B:269:LEU:HD13	1:B:371:PHE:CD1	2.53	0.43
1:C:276:VAL:HG21	1:C:380:ALA:HB3	2.00	0.43
1:C:38:GLN:OE1	1:C:38:GLN:HA	2.18	0.43
1:C:85:VAL:HG12	1:C:197:THR:CG2	2.48	0.43
1:E:391:PHE:O	1:E:394:ARG:HB3	2.18	0.43
1:F:263:ASN:HB2	1:F:298:ILE:HB	1.99	0.43
1:F:446:VAL:HA	1:F:558:VAL:O	2.18	0.43
1:F:95:HIS:O	1:F:98:HIS:HB3	2.17	0.43
1:A:176:ARG:NH2	1:A:609:VAL:O	2.51	0.43
1:B:167:TRP:CZ3	1:B:232:GLU:HG3	2.53	0.43
1:C:433:LEU:HD11	1:C:544:LEU:HD12	2.00	0.43
1:C:502:GLY:O	1:C:503:GLU:C	2.56	0.43
1:D:532:VAL:C	1:D:534:ASN:H	2.21	0.43
1:E:105:ALA:O	1:E:109:ILE:HG13	2.18	0.43
1:E:263:ASN:HB2	1:E:298:ILE:HB	2.00	0.43
1:F:29:THR:CG2	1:F:31:TRP:HE3	2.32	0.43
1:A:158:ASN:HD21	1:A:163:LYS:HB3	1.83	0.43
1:A:193:SER:HB3	1:A:219:VAL:HG13	1.99	0.43
1:A:251:GLY:O	1:A:405:LYS:CG	2.67	0.43
1:A:360:HIS:HE1	1:B:161:TYR:OH	2.00	0.43
1:B:202:HIS:HB3	1:B:205:CYS:SG	2.58	0.43
1:B:459:ASP:HB3	1:B:485:ALA:HB1	1.99	0.43
1:C:33:ARG:NH1	1:D:71:VAL:O	2.52	0.43
1:D:274:CYS:SG	1:D:295:ILE:HD11	2.58	0.43
1:E:532:VAL:C	1:E:534:ASN:H	2.21	0.43
1:F:561:ALA:HB1	1:F:564:CYS:HB3	2.00	0.43
1:F:80:VAL:HG13	1:F:590:PRO:O	2.18	0.43
1:F:62:PRO:HA	1:F:76:ARG:NH2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG23	1:A:229:LEU:HG	1.99	0.43
1:A:309:HIS:ND1	1:A:309:HIS:N	2.66	0.43
1:B:587:SER:O	1:B:588:VAL:HB	2.18	0.43
1:C:255:ARG:NH1	1:C:255:ARG:HG2	2.32	0.43
1:C:587:SER:O	1:C:588:VAL:HB	2.18	0.43
1:D:105:ALA:O	1:D:109:ILE:HG13	2.17	0.43
1:E:152:THR:HG23	1:E:229:LEU:HG	1.99	0.43
1:E:76:ARG:O	1:E:80:VAL:HG23	2.19	0.43
1:E:95:HIS:O	1:E:98:HIS:HB3	2.18	0.43
1:F:250:LEU:C	1:F:252:VAL:N	2.71	0.43
1:A:262:VAL:O	1:A:262:VAL:HG23	2.18	0.43
1:A:29:THR:HG21	1:A:31:TRP:HE3	1.83	0.43
1:A:430:LEU:O	1:A:434:VAL:HG23	2.18	0.43
1:A:459:ASP:HB3	1:A:485:ALA:HB1	2.00	0.43
1:B:110:SER:CA	1:B:145:VAL:HG23	2.48	0.43
1:B:447:LEU:HD13	1:B:449:VAL:CG1	2.49	0.43
1:B:532:VAL:C	1:B:534:ASN:H	2.22	0.43
1:D:471:LYS:C	1:D:473:ASN:H	2.22	0.43
1:E:187:PRO:HD3	1:E:221:MET:HB2	1.99	0.43
1:E:176:ARG:NH1	1:E:551:ASP:OD1	2.51	0.43
1:E:560:SER:C	1:E:562:PRO:HD3	2.39	0.43
1:E:87:MET:O	1:E:567:GLU:HB3	2.18	0.43
1:F:548:LEU:HB2	1:F:550:VAL:HG12	2.01	0.43
1:A:29:THR:CG2	1:A:31:TRP:HE3	2.32	0.43
1:A:322:LEU:N	1:A:322:LEU:HD22	2.32	0.43
1:A:358:ASP:OD1	1:A:360:HIS:N	2.44	0.43
1:A:424:VAL:O	1:A:425:ASN:HB2	2.17	0.43
1:C:310:GLY:O	1:C:311:VAL:C	2.56	0.43
1:C:326:THR:CG2	1:C:328:ALA:HB3	2.49	0.43
1:D:109:ILE:CD1	1:D:237:LEU:HD21	2.48	0.43
1:D:121:ASP:OD2	1:D:240:THR:CG2	2.66	0.43
1:D:76:ARG:O	1:D:80:VAL:HG23	2.19	0.43
1:E:316:ASN:HB2	1:E:317:TYR:H	1.60	0.43
1:F:217:LEU:O	1:F:220:ALA:HB3	2.18	0.43
1:A:229:LEU:HD23	1:A:229:LEU:C	2.39	0.43
1:A:263:ASN:HB2	1:A:298:ILE:HB	2.01	0.43
1:A:327:GLY:O	1:A:394:ARG:HD3	2.18	0.43
1:A:471:LYS:C	1:A:473:ASN:H	2.22	0.43
1:B:425:ASN:HD22	1:B:427:ASP:H	1.66	0.43
1:B:552:LEU:C	1:B:554:ASP:H	2.22	0.43
1:C:570:LEU:HA	1:C:570:LEU:HD12	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:THR:HG23	1:E:495:GLU:OE2	2.17	0.43
1:A:105:ALA:O	1:A:109:ILE:HG13	2.19	0.43
1:A:307:MET:HG3	1:A:529:GLY:HA2	2.00	0.43
1:A:532:VAL:C	1:A:534:ASN:H	2.22	0.43
1:A:71:VAL:HG13	1:B:34:TYR:HB2	2.00	0.43
1:B:471:LYS:C	1:B:473:ASN:H	2.22	0.43
1:B:499:GLN:HG2	1:B:499:GLN:O	2.19	0.43
1:C:446:VAL:HA	1:C:558:VAL:O	2.19	0.43
1:D:96:SER:CB	1:D:190:ILE:HG21	2.49	0.43
1:D:29:THR:CG2	1:D:31:TRP:HE3	2.31	0.43
1:E:424:VAL:O	1:E:425:ASN:HB2	2.18	0.43
1:F:109:ILE:CD1	1:F:237:LEU:HD21	2.49	0.43
1:F:337:GLN:HB3	1:F:337:GLN:HE21	1.61	0.43
1:F:358:ASP:OD1	1:F:360:HIS:N	2.43	0.43
1:A:29:THR:HG22	1:A:32:HIS:CD2	2.54	0.43
1:A:38:GLN:OE1	1:A:40:GLN:HG3	2.19	0.43
1:A:424:VAL:HG13	1:A:432:PRO:HG3	2.00	0.43
1:B:152:THR:HG23	1:B:229:LEU:HG	2.00	0.43
1:C:29:THR:CG2	1:C:31:TRP:HE3	2.31	0.43
1:D:278:ALA:O	1:D:281:ARG:HD2	2.19	0.43
1:D:80:VAL:HG13	1:D:590:PRO:O	2.19	0.43
1:E:158:ASN:HD21	1:E:163:LYS:HB3	1.83	0.43
1:E:202:HIS:CE1	1:F:566:SER:HB2	2.54	0.43
1:E:71:VAL:O	1:F:33:ARG:NH1	2.52	0.43
1:A:499:GLN:HG2	1:A:499:GLN:O	2.19	0.43
1:B:109:ILE:HD12	1:B:237:LEU:HD21	2.01	0.43
1:B:105:ALA:O	1:B:109:ILE:HG13	2.18	0.43
1:B:85:VAL:HG12	1:B:197:THR:CG2	2.48	0.43
1:C:307:MET:HG3	1:C:529:GLY:HA2	2.00	0.43
1:C:421:LEU:HB3	1:C:429:PRO:O	2.18	0.43
1:C:471:LYS:C	1:C:473:ASN:H	2.23	0.43
1:D:187:PRO:HD3	1:D:221:MET:HB2	1.99	0.43
1:D:548:LEU:HB2	1:D:550:VAL:HG12	2.01	0.43
1:E:147:ASP:O	1:E:151:ILE:HG13	2.19	0.43
1:E:402:PRO:HB3	1:E:404:PHE:CD2	2.54	0.43
1:E:38:GLN:OE1	1:E:40:GLN:HG3	2.19	0.43
1:F:117:TYR:CE2	1:F:268:MET:HG2	2.54	0.43
1:F:197:THR:OG1	1:F:219:VAL:HG21	2.19	0.43
1:F:340:MET:HA	1:F:341:PRO:HD3	1.86	0.43
1:A:125:LEU:HD21	1:A:141:LEU:CD1	2.49	0.42
1:A:119:ILE:HG22	1:A:125:LEU:HD22	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD21	1:A:214:LEU:HD22	2.01	0.42
1:A:560:SER:C	1:A:562:PRO:HD3	2.40	0.42
1:B:132:LEU:CD2	1:B:151:ILE:HD13	2.29	0.42
1:B:503:GLU:O	1:B:504:GLY:C	2.57	0.42
1:B:62:PRO:HA	1:B:76:ARG:NH2	2.34	0.42
1:D:322:LEU:HD22	1:D:322:LEU:N	2.33	0.42
1:D:62:PRO:HA	1:D:76:ARG:HH22	1.83	0.42
1:E:224:LEU:HD22	1:E:228:MET:HG3	2.00	0.42
1:F:38:GLN:HA	1:F:38:GLN:OE1	2.18	0.42
1:F:421:LEU:HB3	1:F:429:PRO:O	2.19	0.42
1:A:117:TYR:HE2	1:A:272:ILE:CG1	2.32	0.42
1:A:346:ILE:HD12	1:A:346:ILE:H	1.84	0.42
1:B:158:ASN:ND2	1:B:163:LYS:HE3	2.34	0.42
1:B:276:VAL:O	1:B:279:ASP:HB2	2.20	0.42
1:C:62:PRO:HA	1:C:76:ARG:NH2	2.35	0.42
1:C:76:ARG:O	1:C:80:VAL:HG23	2.18	0.42
1:D:102:ILE:HG23	1:D:237:LEU:HD12	2.01	0.42
1:E:319:SER:HA	1:E:322:LEU:CD2	2.46	0.42
1:E:340:MET:HA	1:E:341:PRO:HD3	1.87	0.42
1:E:38:GLN:OE1	1:E:38:GLN:HA	2.18	0.42
1:E:544:LEU:CD2	1:E:544:LEU:C	2.88	0.42
1:E:62:PRO:HA	1:E:76:ARG:NH2	2.34	0.42
1:F:62:PRO:HG2	1:F:63:PHE:H	1.82	0.42
1:A:109:ILE:HD12	1:A:237:LEU:HD21	2.02	0.42
1:A:119:ILE:CG2	1:A:125:LEU:HD22	2.49	0.42
1:A:567:GLU:OE2	1:B:86:ARG:NH2	2.53	0.42
1:B:29:THR:CG2	1:B:31:TRP:HE3	2.32	0.42
1:C:327:GLY:O	1:C:394:ARG:HD3	2.20	0.42
1:C:424:VAL:O	1:C:425:ASN:HB2	2.19	0.42
1:C:176:ARG:NH1	1:C:551:ASP:OD1	2.53	0.42
1:C:95:HIS:O	1:C:98:HIS:HB3	2.18	0.42
1:E:149:ALA:O	1:E:153:LEU:HB2	2.20	0.42
1:F:319:SER:O	1:F:323:PRO:HD3	2.20	0.42
1:F:501:ALA:O	1:F:506:LYS:HE3	2.19	0.42
1:F:636:GLY:O	1:F:637:LEU:HD23	2.19	0.42
1:A:159:GLN:HB3	1:B:104:LEU:HD21	2.00	0.42
1:A:296:ILE:HD12	1:A:314:ALA:CB	2.50	0.42
1:B:307:MET:HG3	1:B:529:GLY:HA2	1.99	0.42
1:B:29:THR:HG22	1:B:32:HIS:CD2	2.54	0.42
1:B:424:VAL:HG13	1:B:432:PRO:HG3	2.01	0.42
1:B:457:GLN:O	1:B:458:GLN:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:LEU:HB2	1:B:550:VAL:HG12	2.00	0.42
1:C:126:TYR:O	1:C:129:ALA:HB3	2.18	0.42
1:E:424:VAL:CG1	1:E:432:PRO:HG3	2.50	0.42
1:F:117:TYR:HE2	1:F:268:MET:HG2	1.85	0.42
1:F:307:MET:HG3	1:F:529:GLY:HA2	2.01	0.42
1:B:38:GLN:OE1	1:B:40:GLN:HG3	2.19	0.42
1:D:601:VAL:HG23	1:D:602:THR:HG23	2.01	0.42
1:E:102:ILE:HG23	1:E:237:LEU:HD12	2.00	0.42
1:E:309:HIS:N	1:E:309:HIS:ND1	2.68	0.42
1:E:459:ASP:HB3	1:E:485:ALA:HB1	2.00	0.42
1:F:244:VAL:HG22	1:F:245:VAL:N	2.35	0.42
1:F:532:VAL:C	1:F:534:ASN:H	2.22	0.42
1:A:501:ALA:O	1:A:506:LYS:HE3	2.19	0.42
1:B:263:ASN:HB2	1:B:298:ILE:HB	2.02	0.42
1:B:322:LEU:N	1:B:322:LEU:HD22	2.33	0.42
1:B:430:LEU:O	1:B:434:VAL:HG23	2.19	0.42
1:C:187:PRO:HD3	1:C:221:MET:HB2	2.00	0.42
1:C:85:VAL:CG1	1:C:197:THR:HG23	2.49	0.42
1:E:109:ILE:HD12	1:E:237:LEU:HD21	2.02	0.42
1:E:430:LEU:O	1:E:434:VAL:HG23	2.20	0.42
1:E:552:LEU:C	1:E:554:ASP:H	2.22	0.42
1:E:601:VAL:HG23	1:E:602:THR:HG23	2.01	0.42
1:F:100:ARG:HH12	1:F:191:ASP:CG	2.23	0.42
1:F:149:ALA:O	1:F:153:LEU:HB2	2.19	0.42
1:F:326:THR:CG2	1:F:328:ALA:HB3	2.50	0.42
1:F:450:GLY:O	4:F:800:WCC:S1	2.77	0.42
1:A:556:PRO:HB2	1:A:630:ILE:HG23	2.01	0.42
1:B:498:THR:HA	1:B:506:LYS:HE2	2.02	0.42
1:C:260:ILE:O	1:C:295:ILE:HA	2.18	0.42
1:D:185:LEU:HD21	1:D:214:LEU:HD22	2.01	0.42
1:D:501:ALA:O	1:D:506:LYS:HB2	2.19	0.42
1:A:119:ILE:O	1:A:121:ASP:N	2.53	0.42
1:A:132:LEU:HD12	1:A:148:LEU:CD2	2.48	0.42
1:A:446:VAL:O	1:A:446:VAL:HG13	2.20	0.42
1:B:96:SER:CB	1:B:190:ILE:HG21	2.49	0.42
1:B:319:SER:O	1:B:323:PRO:HD3	2.19	0.42
1:D:152:THR:HG23	1:D:229:LEU:HG	2.02	0.42
1:D:459:ASP:HB3	1:D:485:ALA:HB1	2.01	0.42
1:E:260:ILE:O	1:E:295:ILE:HA	2.19	0.42
1:E:422:ALA:C	1:E:424:VAL:H	2.23	0.42
1:F:552:LEU:C	1:F:554:ASP:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:N	1:B:134:VAL:HG21	2.35	0.42
1:C:38:GLN:OE1	1:C:40:GLN:HG3	2.19	0.42
1:D:402:PRO:HB3	1:D:404:PHE:CD2	2.54	0.42
1:F:309:HIS:N	1:F:309:HIS:ND1	2.67	0.42
1:F:430:LEU:O	1:F:434:VAL:HG23	2.20	0.42
1:F:501:ALA:O	1:F:506:LYS:HB2	2.19	0.42
1:B:326:THR:CG2	1:B:328:ALA:HB3	2.49	0.42
1:B:326:THR:CG2	1:B:401:ILE:HG12	2.50	0.42
1:B:372:ASP:CB	1:B:375:LYS:HZ2	2.25	0.42
1:C:282:ASP:C	1:C:284:ALA:N	2.72	0.42
1:C:319:SER:O	1:C:323:PRO:HD3	2.19	0.42
1:C:501:ALA:O	1:C:506:LYS:HE3	2.20	0.42
1:D:110:SER:HB3	1:D:145:VAL:HG12	2.01	0.42
1:E:144:ILE:O	1:E:146:GLY:N	2.53	0.42
1:E:296:ILE:HD12	1:E:314:ALA:CB	2.49	0.42
1:E:471:LYS:C	1:E:473:ASN:H	2.23	0.42
1:E:503:GLU:O	1:E:504:GLY:C	2.58	0.42
1:A:552:LEU:HD12	1:A:552:LEU:H	1.85	0.41
1:A:601:VAL:HG23	1:A:602:THR:HG23	2.02	0.41
1:B:102:ILE:HG23	1:B:237:LEU:HD12	2.01	0.41
1:B:140:GLY:O	1:B:143:ALA:HB3	2.20	0.41
1:B:71:VAL:HG12	1:B:71:VAL:O	2.20	0.41
1:D:499:GLN:HG2	1:D:499:GLN:O	2.20	0.41
1:D:552:LEU:C	1:D:554:ASP:H	2.24	0.41
1:B:111:GLN:NE2	1:B:113:GLU:OE2	2.53	0.41
1:B:424:VAL:O	1:B:425:ASN:HB2	2.19	0.41
1:B:501:ALA:O	1:B:506:LYS:HB2	2.20	0.41
1:B:522:LEU:HD13	1:B:526:MET:CE	2.28	0.41
1:C:119:ILE:N	1:C:119:ILE:HD13	2.35	0.41
1:C:158:ASN:ND2	1:C:163:LYS:HE3	2.35	0.41
1:D:132:LEU:HD22	1:D:132:LEU:HA	1.93	0.41
1:D:62:PRO:HG2	1:D:63:PHE:H	1.85	0.41
1:D:62:PRO:HA	1:D:76:ARG:NH2	2.35	0.41
1:F:327:GLY:O	1:F:394:ARG:HD3	2.20	0.41
1:F:422:ALA:C	1:F:424:VAL:H	2.24	0.41
1:B:319:SER:HA	1:B:322:LEU:CD2	2.46	0.41
1:C:309:HIS:N	1:C:309:HIS:ND1	2.68	0.41
1:D:431:LYS:N	1:D:432:PRO:HD2	2.35	0.41
1:F:324:ILE:HD11	1:F:343:LEU:HD12	2.01	0.41
1:A:402:PRO:HB3	1:A:404:PHE:CD2	2.55	0.41
1:A:502:GLY:O	1:A:503:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:CD2	1:B:151:ILE:HG21	2.50	0.41
1:B:62:PRO:HG2	1:B:63:PHE:H	1.85	0.41
1:C:109:ILE:HD12	1:C:237:LEU:HD21	2.02	0.41
1:C:552:LEU:C	1:C:554:ASP:H	2.24	0.41
1:D:106:MET:CE	1:D:233:LEU:HD22	2.50	0.41
1:D:260:ILE:O	1:D:295:ILE:HA	2.19	0.41
1:E:421:LEU:HB3	1:E:429:PRO:O	2.21	0.41
1:E:548:LEU:HB2	1:E:550:VAL:HG12	2.02	0.41
1:F:167:TRP:CZ3	1:F:232:GLU:HG3	2.55	0.41
1:F:317:TYR:CE2	1:F:565:MET:HE1	2.56	0.41
1:F:316:ASN:HB2	1:F:317:TYR:H	1.61	0.41
1:A:106:MET:CE	1:A:233:LEU:HD22	2.51	0.41
1:B:130:LYS:C	1:B:132:LEU:N	2.74	0.41
1:B:127:ALA:HA	1:B:130:LYS:CG	2.50	0.41
1:B:560:SER:C	1:B:562:PRO:HD3	2.41	0.41
1:C:167:TRP:CZ3	1:C:232:GLU:HG3	2.56	0.41
1:C:503:GLU:O	1:C:504:GLY:C	2.58	0.41
1:D:319:SER:HA	1:D:322:LEU:CD2	2.47	0.41
1:D:424:VAL:HG13	1:D:432:PRO:HG3	2.02	0.41
1:D:636:GLY:O	1:D:637:LEU:HD23	2.21	0.41
1:E:250:LEU:C	1:E:252:VAL:N	2.74	0.41
1:A:266:ASN:HA	1:A:267:PRO:HD2	1.98	0.41
1:A:326:THR:CG2	1:A:401:ILE:HG12	2.51	0.41
1:A:422:ALA:C	1:A:424:VAL:H	2.24	0.41
1:B:402:PRO:HB3	1:B:404:PHE:CD2	2.55	0.41
1:B:422:ALA:C	1:B:424:VAL:H	2.23	0.41
1:B:544:LEU:C	1:B:544:LEU:CD2	2.89	0.41
1:B:636:GLY:O	1:B:637:LEU:HD23	2.21	0.41
1:C:326:THR:CG2	1:C:401:ILE:HG12	2.50	0.41
1:C:335:ASP:CG	1:C:336:VAL:N	2.74	0.41
1:F:124:LYS:NZ	1:F:235:ASP:HB2	2.36	0.41
1:F:447:LEU:HD13	1:F:449:VAL:CG1	2.50	0.41
1:A:424:VAL:CG1	1:A:432:PRO:HG3	2.51	0.41
1:A:447:LEU:HD13	1:A:449:VAL:CG1	2.50	0.41
1:B:251:GLY:HA2	1:B:402:PRO:O	2.21	0.41
1:B:421:LEU:HB3	1:B:429:PRO:O	2.19	0.41
1:C:422:ALA:C	1:C:424:VAL:H	2.23	0.41
1:C:472:ARG:HH11	1:C:472:ARG:CG	2.29	0.41
1:D:424:VAL:O	1:D:425:ASN:HB2	2.20	0.41
1:D:503:GLU:O	1:D:504:GLY:C	2.58	0.41
1:D:560:SER:C	1:D:562:PRO:HD3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:TYR:O	1:E:118:SER:HB3	2.21	0.41
1:E:29:THR:HG21	1:E:31:TRP:HE3	1.85	0.41
1:E:80:VAL:HG13	1:E:590:PRO:O	2.21	0.41
1:F:158:ASN:HD21	1:F:163:LYS:HB3	1.85	0.41
1:F:296:ILE:HD12	1:F:314:ALA:CB	2.51	0.41
1:F:499:GLN:HG2	1:F:499:GLN:O	2.21	0.41
1:F:560:SER:C	1:F:562:PRO:HD3	2.40	0.41
1:F:71:VAL:HG12	1:F:71:VAL:O	2.19	0.41
1:F:99:GLY:O	1:F:100:ARG:C	2.58	0.41
1:A:168:LEU:HD22	1:A:172:LEU:HD11	2.03	0.41
1:A:102:ILE:HG23	1:A:237:LEU:HD12	2.01	0.41
1:A:274:CYS:SG	1:A:295:ILE:HD11	2.61	0.41
1:A:514:THR:C	1:A:516:ALA:H	2.23	0.41
1:A:544:LEU:CD2	1:A:544:LEU:C	2.89	0.41
1:B:108:HIS:HB2	1:B:114:LEU:CD1	2.49	0.41
1:B:127:ALA:CA	1:B:130:LYS:HZ3	2.15	0.41
1:C:431:LYS:N	1:C:432:PRO:HD2	2.36	0.41
1:D:224:LEU:HD22	1:D:228:MET:HG3	2.02	0.41
1:D:276:VAL:HG22	1:D:377:VAL:HG13	2.03	0.41
1:D:430:LEU:O	1:D:434:VAL:HG23	2.20	0.41
1:D:534:ASN:HD22	1:D:572:ILE:HD13	1.85	0.41
1:F:167:TRP:HB3	1:F:228:MET:HE3	2.01	0.41
1:F:250:LEU:C	1:F:252:VAL:H	2.23	0.41
1:B:168:LEU:HD22	1:B:172:LEU:HD11	2.03	0.41
1:C:340:MET:HA	1:C:341:PRO:HD3	1.87	0.41
1:D:229:LEU:C	1:D:229:LEU:HD23	2.41	0.41
1:D:38:GLN:OE1	1:D:38:GLN:HA	2.20	0.41
1:E:167:TRP:HB3	1:E:228:MET:CE	2.51	0.41
1:E:501:ALA:O	1:E:506:LYS:HB2	2.20	0.41
1:E:71:VAL:HG12	1:E:71:VAL:O	2.21	0.41
1:F:317:TYR:CE2	1:F:565:MET:CE	3.04	0.41
1:F:424:VAL:CG1	1:F:432:PRO:HG3	2.50	0.41
1:A:129:ALA:HB1	1:A:134:VAL:HB	2.02	0.41
1:A:552:LEU:C	1:A:554:ASP:H	2.23	0.41
1:B:127:ALA:O	1:B:128:ILE:HG23	2.21	0.41
1:B:424:VAL:CG1	1:B:432:PRO:HG3	2.51	0.41
1:C:424:VAL:CG1	1:C:432:PRO:HG3	2.51	0.41
1:C:534:ASN:HD22	1:C:572:ILE:HD13	1.85	0.41
1:D:109:ILE:HD12	1:D:237:LEU:HD21	2.03	0.41
1:D:340:MET:HA	1:D:341:PRO:HD3	1.86	0.41
1:D:324:ILE:HD11	1:D:343:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:LEU:HD22	1:F:228:MET:HG3	2.02	0.41
1:A:319:SER:O	1:A:323:PRO:HD3	2.20	0.41
1:A:324:ILE:HD11	1:A:343:LEU:HD12	2.03	0.41
1:B:124:LYS:HE2	1:B:235:ASP:CB	2.50	0.41
1:B:149:ALA:O	1:B:153:LEU:HB2	2.21	0.41
1:C:544:LEU:C	1:C:544:LEU:CD2	2.89	0.41
1:D:167:TRP:CZ3	1:D:232:GLU:HG3	2.55	0.41
1:D:255:ARG:CZ	1:D:399:VAL:HB	2.47	0.41
1:D:544:LEU:C	1:D:544:LEU:CD2	2.89	0.41
1:D:50:CYS:HB2	1:D:79:ILE:HG23	2.01	0.41
1:E:31:TRP:CZ3	1:E:322:LEU:HD21	2.56	0.41
1:F:281:ARG:O	1:F:285:ILE:HG13	2.20	0.41
1:F:534:ASN:O	1:F:538:VAL:HG23	2.21	0.41
1:F:587:SER:O	1:F:588:VAL:HB	2.20	0.41
1:A:109:ILE:C	1:A:111:GLN:H	2.24	0.40
1:B:141:LEU:O	1:B:143:ALA:N	2.50	0.40
1:C:425:ASN:ND2	1:C:425:ASN:C	2.73	0.40
1:F:102:ILE:HG23	1:F:237:LEU:HD12	2.02	0.40
1:F:503:GLU:O	1:F:504:GLY:C	2.59	0.40
1:F:601:VAL:HG23	1:F:602:THR:HG23	2.03	0.40
1:B:108:HIS:HB3	1:B:113:GLU:HG3	2.02	0.40
1:B:431:LYS:N	1:B:432:PRO:HD2	2.36	0.40
1:D:307:MET:HG3	1:D:529:GLY:HA2	2.02	0.40
1:D:309:HIS:N	1:D:309:HIS:ND1	2.68	0.40
1:E:433:LEU:HD11	1:E:544:LEU:HD12	2.02	0.40
1:F:144:ILE:H	1:F:144:ILE:HD12	1.86	0.40
1:F:425:ASN:C	1:F:425:ASN:ND2	2.74	0.40
1:A:124:LYS:HD3	1:A:235:ASP:CB	2.51	0.40
1:B:296:ILE:HD12	1:B:314:ALA:CB	2.51	0.40
1:B:513:GLY:O	1:B:518:LEU:HD11	2.21	0.40
1:A:34:TYR:HB2	1:B:71:VAL:HG13	2.02	0.40
1:C:202:HIS:HB3	1:C:205:CYS:SG	2.60	0.40
1:C:29:THR:HG22	1:C:32:HIS:CD2	2.56	0.40
1:E:29:THR:HG22	1:E:32:HIS:CD2	2.56	0.40
1:E:276:VAL:HG22	1:E:377:VAL:HG13	2.03	0.40
1:E:556:PRO:HB2	1:E:630:ILE:HG23	2.03	0.40
1:F:140:GLY:O	1:F:143:ALA:HB3	2.21	0.40
1:F:283:GLU:O	1:F:286:ALA:HB3	2.22	0.40
1:F:269:LEU:HD13	1:F:371:PHE:CD1	2.57	0.40
1:A:110:SER:HB3	1:A:145:VAL:CG1	2.43	0.40
1:A:326:THR:HG22	1:A:328:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:PHE:N	1:A:350:PHE:CD1	2.90	0.40
1:B:168:LEU:HA	1:B:228:MET:HE1	2.04	0.40
1:C:141:LEU:C	1:C:143:ALA:N	2.73	0.40
1:E:85:VAL:HG12	1:E:197:THR:HG23	2.01	0.40
1:F:476:VAL:HG12	1:F:525:VAL:HG13	2.03	0.40
1:A:503:GLU:O	1:A:504:GLY:C	2.59	0.40
1:A:548:LEU:HB2	1:A:550:VAL:HG12	2.02	0.40
1:C:224:LEU:HD22	1:C:228:MET:CG	2.51	0.40
1:D:132:LEU:CD1	1:D:151:ILE:HG21	2.33	0.40
1:C:566:SER:HB2	1:D:202:HIS:CE1	2.56	0.40
1:D:457:GLN:O	1:D:458:GLN:C	2.59	0.40
1:E:581:LEU:HA	1:E:582:PRO:HD3	1.99	0.40
1:F:492:MET:CE	1:F:527:HIS:HB2	2.51	0.40
1:F:556:PRO:HB2	1:F:630:ILE:HG23	2.03	0.40
1:F:53:CYS:SG	1:F:55:LYS:HB2	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	608/639 (95%)	523 (86%)	69 (11%)	16 (3%)	6	21
1	B	608/639 (95%)	510 (84%)	79 (13%)	19 (3%)	5	16
1	C	608/639 (95%)	535 (88%)	58 (10%)	15 (2%)	6	22
1	D	608/639 (95%)	535 (88%)	64 (10%)	9 (2%)	12	37
1	E	608/639 (95%)	530 (87%)	66 (11%)	12 (2%)	9	28
1	F	608/639 (95%)	537 (88%)	56 (9%)	15 (2%)	6	22
All	All	3648/3834 (95%)	3170 (87%)	392 (11%)	86 (2%)	7	23

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	GLY
1	A	141	LEU
1	A	337	GLN
1	A	425	ASN
1	A	458	GLN
1	B	64	GLY
1	B	280	LEU
1	B	337	GLN
1	B	425	ASN
1	B	458	GLN
1	C	64	GLY
1	C	337	GLN
1	C	425	ASN
1	C	458	GLN
1	D	64	GLY
1	D	337	GLN
1	D	425	ASN
1	D	458	GLN
1	E	64	GLY
1	E	141	LEU
1	E	337	GLN
1	E	425	ASN
1	E	458	GLN
1	F	64	GLY
1	F	337	GLN
1	F	425	ASN
1	F	458	GLN
1	A	120	ARG
1	A	142	LEU
1	A	519	GLY
1	B	130	LYS
1	B	282	ASP
1	C	517	GLY
1	D	114	LEU
1	E	114	LEU
1	F	250	LEU
1	B	128	ILE
1	B	137	GLU
1	B	142	LEU
1	B	145	VAL
1	C	280	LEU
1	E	280	LEU
1	E	423	LYS

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Mol	Chain	Res	Type
1	F	114	LEU
1	A	252	VAL
1	A	423	LYS
1	B	423	LYS
1	C	142	LEU
1	C	283	GLU
1	C	423	LYS
1	C	506	LYS
1	D	423	LYS
1	E	519	GLY
1	F	141	LEU
1	F	249	ASN
1	F	423	LYS
1	A	116	ASP
1	A	503	GLU
1	A	506	LYS
1	B	506	LYS
1	B	518	LEU
1	C	503	GLU
1	E	506	LYS
1	F	472	ARG
1	F	506	LYS
1	A	376	ALA
1	B	120	ARG
1	B	503	GLU
1	B	590	PRO
1	C	376	ALA
1	D	376	ALA
1	D	590	PRO
1	F	376	ALA
1	F	503	GLU
1	A	588	VAL
1	B	252	VAL
1	C	590	PRO
1	E	588	VAL
1	E	590	PRO
1	A	590	PRO
1	B	588	VAL
1	D	588	VAL
1	F	590	PRO
1	C	119	ILE
1	C	588	VAL

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Mol	Chain	Res	Type
1	F	588	VAL

### 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	466/490 (95%)	438 (94%)	28 (6%)	22	54
1	B	466/490 (95%)	433 (93%)	33 (7%)	17	44
1	C	466/490 (95%)	436 (94%)	30 (6%)	20	50
1	D	466/490 (95%)	432 (93%)	34 (7%)	16	42
1	E	466/490 (95%)	433 (93%)	33 (7%)	17	44
1	F	466/490 (95%)	437 (94%)	29 (6%)	21	52
All	All	2796/2940 (95%)	2609 (93%)	187 (7%)	19	48

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	63	PHE
1	A	84	LEU
1	A	115	HIS
1	A	126	TYR
1	A	176	ARG
1	A	224	LEU
1	A	229	LEU
1	A	240	THR
1	A	242	GLN
1	A	316	ASN
1	A	319	SER
1	A	330	GLU
1	A	337	GLN
1	A	385	ARG
1	A	394	ARG
1	A	423	LYS

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Mol	Chain	Res	Type
1	A	425	ASN
1	A	447	LEU
1	A	458	GLN
1	A	465	LEU
1	A	472	ARG
1	A	495	GLU
1	A	508	VAL
1	A	509	LEU
1	A	540	LEU
1	A	587	SER
1	A	620	LYS
1	B	29	THR
1	B	63	PHE
1	B	84	LEU
1	B	117	TYR
1	B	124	LYS
1	B	130	LYS
1	B	132	LEU
1	B	144	ILE
1	B	176	ARG
1	B	224	LEU
1	B	229	LEU
1	B	240	THR
1	B	242	GLN
1	B	280	LEU
1	B	281	ARG
1	B	309	HIS
1	B	316	ASN
1	B	319	SER
1	B	330	GLU
1	B	337	GLN
1	B	385	ARG
1	B	394	ARG
1	B	423	LYS
1	B	425	ASN
1	B	447	LEU
1	B	458	GLN
1	B	465	LEU
1	B	472	ARG
1	B	495	GLU
1	B	508	VAL
1	B	509	LEU

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Mol	Chain	Res	Type
1	B	540	LEU
1	B	620	LYS
1	C	29	THR
1	C	63	PHE
1	C	84	LEU
1	C	124	LYS
1	C	176	ARG
1	C	224	LEU
1	C	229	LEU
1	C	240	THR
1	C	242	GLN
1	C	255	ARG
1	C	282	ASP
1	C	283	GLU
1	C	309	HIS
1	C	319	SER
1	C	330	GLU
1	C	337	GLN
1	C	385	ARG
1	C	394	ARG
1	C	423	LYS
1	C	425	ASN
1	C	447	LEU
1	C	458	GLN
1	C	465	LEU
1	C	472	ARG
1	C	495	GLU
1	C	508	VAL
1	C	509	LEU
1	C	540	LEU
1	C	587	SER
1	C	620	LYS
1	D	29	THR
1	D	63	PHE
1	D	84	LEU
1	D	132	LEU
1	D	139	ARG
1	D	157	GLN
1	D	176	ARG
1	D	224	LEU
1	D	229	LEU
1	D	240	THR

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Mol	Chain	Res	Type
1	D	242	GLN
1	D	252	VAL
1	D	280	LEU
1	D	281	ARG
1	D	316	ASN
1	D	319	SER
1	D	326	THR
1	D	330	GLU
1	D	337	GLN
1	D	385	ARG
1	D	394	ARG
1	D	423	LYS
1	D	425	ASN
1	D	447	LEU
1	D	458	GLN
1	D	465	LEU
1	D	472	ARG
1	D	495	GLU
1	D	508	VAL
1	D	509	LEU
1	D	518	LEU
1	D	540	LEU
1	D	587	SER
1	D	620	LYS
1	E	29	THR
1	E	63	PHE
1	E	84	LEU
1	E	116	ASP
1	E	120	ARG
1	E	125	LEU
1	E	134	VAL
1	E	145	VAL
1	E	176	ARG
1	E	224	LEU
1	E	229	LEU
1	E	240	THR
1	E	242	GLN
1	E	250	LEU
1	E	281	ARG
1	E	316	ASN
1	E	319	SER
1	E	330	GLU

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Mol	Chain	Res	Type
1	E	337	GLN
1	E	385	ARG
1	E	394	ARG
1	E	423	LYS
1	E	425	ASN
1	E	447	LEU
1	E	458	GLN
1	E	465	LEU
1	E	472	ARG
1	E	495	GLU
1	E	508	VAL
1	E	509	LEU
1	E	540	LEU
1	E	587	SER
1	E	620	LYS
1	F	29	THR
1	F	63	PHE
1	F	84	LEU
1	F	118	SER
1	F	121	ASP
1	F	132	LEU
1	F	176	ARG
1	F	224	LEU
1	F	229	LEU
1	F	240	THR
1	F	242	GLN
1	F	282	ASP
1	F	319	SER
1	F	330	GLU
1	F	337	GLN
1	F	385	ARG
1	F	394	ARG
1	F	423	LYS
1	F	425	ASN
1	F	447	LEU
1	F	458	GLN
1	F	465	LEU
1	F	472	ARG
1	F	495	GLU
1	F	508	VAL
1	F	509	LEU
1	F	540	LEU

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Mol	Chain	Res	Type
1	F	587	SER
1	F	620	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	111	GLN
1	A	202	HIS
1	A	211	ASN
1	A	249	ASN
1	A	266	ASN
1	A	337	GLN
1	A	360	HIS
1	A	361	ASN
1	A	425	ASN
1	A	436	ASN
1	A	441	ASN
1	A	452	ASN
1	A	457	GLN
1	A	499	GLN
1	B	40	GLN
1	B	111	GLN
1	B	202	HIS
1	B	266	ASN
1	B	337	GLN
1	B	360	HIS
1	B	361	ASN
1	B	374	HIS
1	B	425	ASN
1	B	436	ASN
1	B	441	ASN
1	B	452	ASN
1	B	457	GLN
1	B	499	GLN
1	C	40	GLN
1	C	111	GLN
1	C	202	HIS
1	C	266	ASN
1	C	337	GLN
1	C	360	HIS
1	C	361	ASN

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Mol	Chain	Res	Type
1	C	425	ASN
1	C	436	ASN
1	C	441	ASN
1	C	452	ASN
1	C	457	GLN
1	C	499	GLN
1	D	40	GLN
1	D	111	GLN
1	D	202	HIS
1	D	266	ASN
1	D	337	GLN
1	D	360	HIS
1	D	361	ASN
1	D	425	ASN
1	D	436	ASN
1	D	441	ASN
1	D	452	ASN
1	D	457	GLN
1	D	499	GLN
1	E	40	GLN
1	E	111	GLN
1	E	202	HIS
1	E	249	ASN
1	E	266	ASN
1	E	337	GLN
1	E	360	HIS
1	E	361	ASN
1	E	425	ASN
1	E	436	ASN
1	E	441	ASN
1	E	452	ASN
1	E	457	GLN
1	E	499	GLN
1	F	40	GLN
1	F	111	GLN
1	F	202	HIS
1	F	266	ASN
1	F	337	GLN
1	F	360	HIS
1	F	361	ASN
1	F	425	ASN
1	F	436	ASN

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Mol	Chain	Res	Type
1	F	441	ASN
1	F	452	ASN
1	F	457	GLN
1	F	499	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 6 are monoatomic and 6 are unknown - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SF4	A	700	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	A	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	WCC	A	800	1,2,5	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	B	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	WCC	B	800	1,2,5	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	C	701	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	C	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	WCC	C	800	1,2,5	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	D	750	1	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	WCC	D	800	1,2,5	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	E	702	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	E	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	WCC	E	800	1,2,5	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	F	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	WCC	F	800	1,2,5	0,12,12	0.00	-	0,24,24	0.00	-

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	SF4	A	700	1	-	0/0/48/48	0/6/5/5
3	SF4	A	750	1	-	0/0/48/48	0/6/5/5
4	WCC	A	800	1,2,5	-	0/0/48/48	0/6/5/5
3	SF4	B	750	1	-	0/0/48/48	0/6/5/5
4	WCC	B	800	1,2,5	-	0/0/48/48	0/6/5/5
3	SF4	C	701	1	-	0/0/48/48	0/6/5/5
3	SF4	C	750	1	-	0/0/48/48	0/6/5/5
4	WCC	C	800	1,2,5	-	0/0/48/48	0/6/5/5
3	SF4	D	750	1	-	0/0/48/48	0/6/5/5
4	WCC	D	800	1,2,5	-	0/0/48/48	0/6/5/5
3	SF4	E	702	1	-	0/0/48/48	0/6/5/5
3	SF4	E	750	1	-	0/0/48/48	0/6/5/5
4	WCC	E	800	1,2,5	-	0/0/48/48	0/6/5/5
3	SF4	F	750	1	-	0/0/48/48	0/6/5/5
4	WCC	F	800	1,2,5	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	WCC	1	0
4	B	800	WCC	1	0
4	C	800	WCC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	800	WCC	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.