



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:58 PM GMT

PDB ID : 2HT3  
Title : Structure of the Escherichia coli ClC chloride channel Y445L mutant and Fab complex  
Authors : Accardi, A.; Lobet, S.; Williams, C.; Miller, C.; Dutzler, R.  
Deposited on : 2006-07-25  
Resolution : 3.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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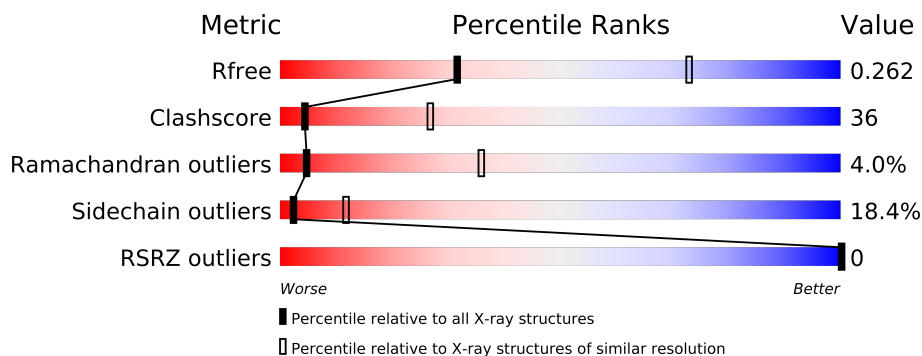
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	473	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
1	B	473	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
2	C	221	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
2	E	221	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
3	D	211	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>
3	F	211	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	BR	A	474	-	X
4	BR	A	475	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	BR	B	474	-	X
4	BR	B	475	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13219 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3329	2187	560	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3300	2171	553	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	LEU	TYR	ENGINEERED	UNP P37019
B	445	LEU	TYR	ENGINEERED	UNP P37019

- Molecule 2 is a protein called Fab fragment, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

- Molecule 3 is a protein called Fab fragment, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Br	0	0
			2	2		

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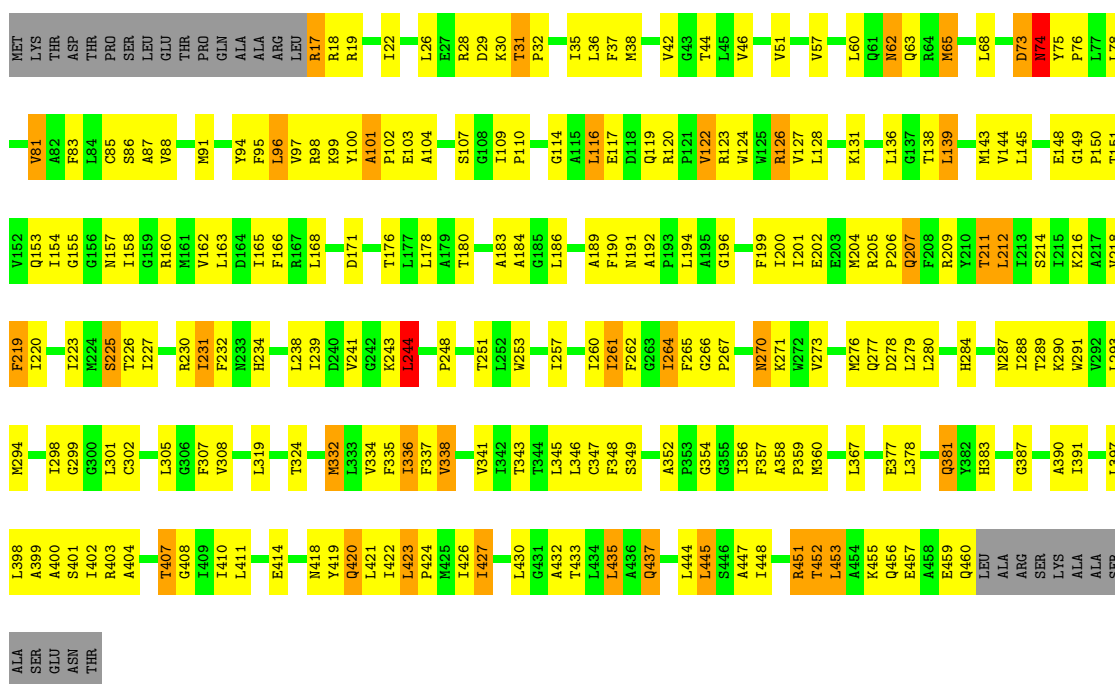
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Br	0	0
			2	2		

### 3 Residue-property plots

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

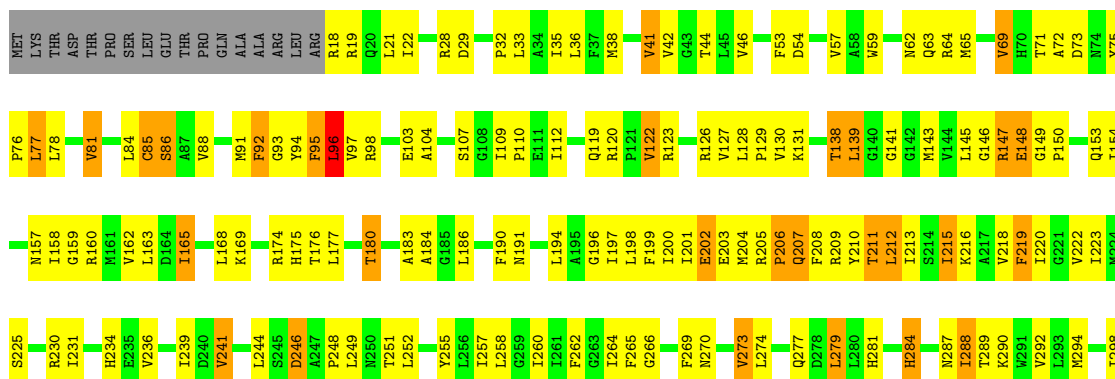
- Molecule 1: H(+)/Cl(-) exchange transporter clcA

Chain A:



- Molecule 1: H(+)/Cl(-) exchange transporter clcA

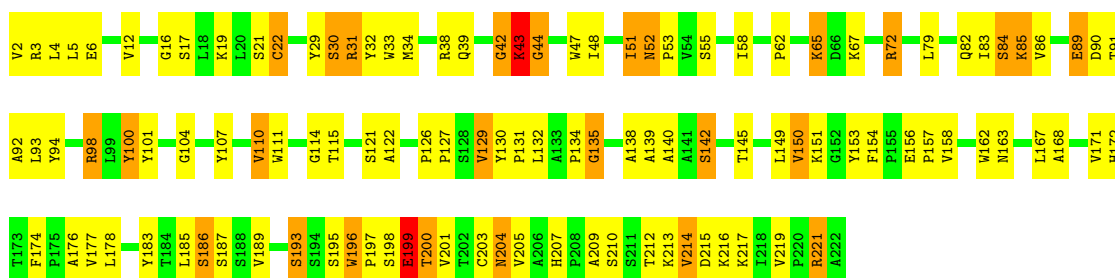
Chain B:





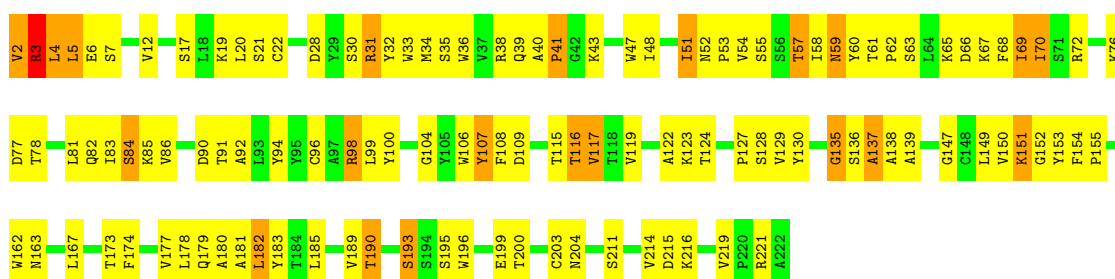
• Molecule 2: Fab fragment, Heavy chain

Chain C:



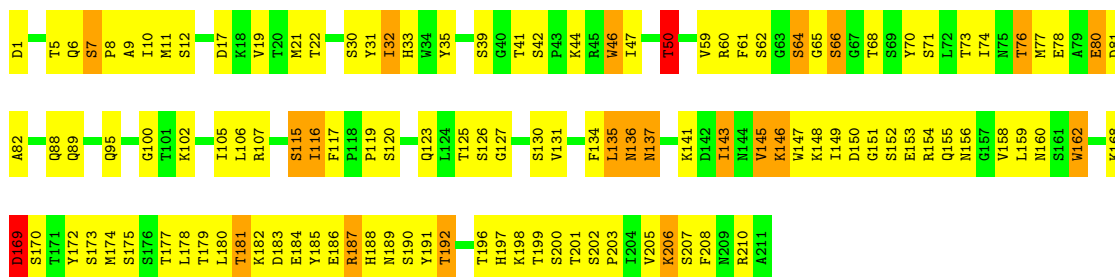
• Molecule 2: Fab fragment, Heavy chain

Chain E:



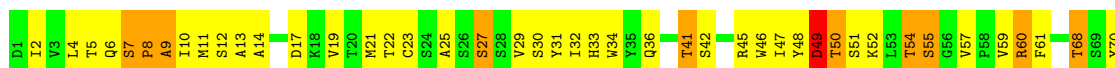
• Molecule 3: Fab fragment, Light chain

Chain D:



• Molecule 3: Fab fragment, Light chain

Chain F:







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	221.63Å 124.85Å 150.72Å 90.00° 128.15° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 19.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-3.30) 98.0 (19.99-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.253 , 0.269 0.246 , 0.262	Depositor DCC
$R_{free}$ test set	2515 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.7	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52979 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR

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	0.72	1/3400 (0.0%)	0.84	4/4614 (0.1%)
1	B	0.74	1/3371 (0.0%)	0.84	4/4576 (0.1%)
2	C	0.74	0/1721	0.90	0/2355
2	E	0.83	0/1721	0.86	0/2355
3	D	0.66	0/1660	0.80	1/2257 (0.0%)
3	F	0.83	0/1660	0.90	1/2257 (0.0%)
All	All	0.75	2/13533 (0.0%)	0.85	10/18414 (0.1%)

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
2	C	0	2
3	F	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	CYS	CB-SG	-7.60	1.69	1.82
1	B	85	CYS	CB-SG	-5.21	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LEU	CA-CB-CG	7.21	131.88	115.30
1	B	212	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	139	LEU	CA-CB-CG	6.35	129.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	135	LEU	CA-CB-CG	6.11	129.34	115.30
1	B	244	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	279	LEU	CA-CB-CG	5.61	128.19	115.30
1	B	78	LEU	CA-CB-CG	5.36	127.62	115.30
3	F	49	ASP	N-CA-C	-5.33	96.60	111.00
1	A	244	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	116	LEU	CB-CG-CD1	-5.07	102.39	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	196	TRP	Peptide
2	C	199	GLU	Peptide
3	F	197	HIS	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3329	0	3486	251	0
1	B	3300	0	3459	268	0
2	C	1672	0	1654	98	0
2	E	1672	0	1654	116	0
3	D	1621	0	1546	122	0
3	F	1621	0	1546	158	0
4	A	2	0	0	3	0
4	B	2	0	0	7	0
All	All	13219	0	13345	945	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (945) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:LYS:HE2	1:B:153:GLN:NE2	1.41	1.33
3:D:95:GLN:N	3:D:95:GLN:OE1	1.63	1.30
1:B:109:ILE:HD12	4:B:474:BR:BR	1.88	1.27
3:D:7:SER:HB3	3:D:8:PRO:CD	1.74	1.17
1:A:453:LEU:HB3	1:B:22:ILE:HD11	1.27	1.16
3:D:82:ALA:HB2	3:D:105:ILE:HD13	1.27	1.16
2:C:150:VAL:HG11	2:C:205:VAL:HG11	1.26	1.15
2:E:17:SER:CB	2:E:84:SER:HA	1.79	1.12
2:E:51:ILE:HD11	2:E:55:SER:HA	1.26	1.11
3:D:7:SER:CB	3:D:8:PRO:HD3	1.80	1.10
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.17	1.10
2:C:51:ILE:HD11	2:C:55:SER:HA	1.32	1.09
3:F:191:TYR:O	3:F:207:SER:HB2	1.51	1.07
2:E:17:SER:HB3	2:E:84:SER:HA	1.31	1.06
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.37	1.06
1:B:93:GLY:O	1:B:97:VAL:HG23	1.54	1.06
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.09	1.05
2:E:60:TYR:HE2	2:E:70:ILE:HD13	1.23	1.04
3:F:7:SER:CB	3:F:8:PRO:HD3	1.90	1.02
3:F:150:ASP:HA	3:F:190:SER:HB3	1.42	1.00
3:D:116:ILE:HD13	3:D:117:PHE:N	1.76	1.00
1:B:206:PRO:HG2	1:B:211:THR:OG1	1.61	1.00
3:F:7:SER:HB2	3:F:22:THR:HB	1.42	1.00
3:F:7:SER:OG	3:F:8:PRO:HD3	1.62	0.99
2:C:100:TYR:HD2	2:C:101:TYR:H	1.01	0.99
1:A:51:VAL:HG11	1:A:232:PHE:CD2	1.97	0.99
1:A:332:MET:O	1:A:336:ILE:HD13	1.63	0.99
1:A:231:ILE:HG22	1:A:232:PHE:CD1	1.97	0.99
3:F:7:SER:HB3	3:F:8:PRO:CD	1.93	0.99
1:B:381:GLN:H	1:B:381:GLN:HE21	1.07	0.99
2:C:16:GLY:O	2:C:86:VAL:HG23	1.60	0.98
1:B:287:ASN:ND2	1:B:290:LYS:H	1.62	0.98
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.26	0.97
1:A:22:ILE:O	1:A:26:LEU:HD12	1.65	0.96
1:A:257:ILE:O	1:A:261:ILE:HD13	1.66	0.96
2:E:60:TYR:CE2	2:E:70:ILE:HD13	2.01	0.96
1:A:51:VAL:HG11	1:A:232:PHE:HD2	1.27	0.95
1:B:391:ILE:HD12	1:B:416:THR:HG21	1.49	0.95
2:E:2:VAL:O	2:E:3:ARG:HB2	1.64	0.95
2:E:58:ILE:O	2:E:58:ILE:HG22	1.66	0.95
3:F:7:SER:CB	3:F:8:PRO:CD	2.45	0.95
1:A:453:LEU:CB	1:B:22:ILE:HD11	1.99	0.92
3:F:146:LYS:HE3	3:F:153:GLU:HG3	1.48	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:131:LYS:HE2	1:B:153:GLN:HE21	1.13	0.92
3:F:49:ASP:HB2	3:F:52:LYS:HE3	1.53	0.91
2:C:142:SER:O	2:C:193:SER:HB2	1.71	0.91
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.02	0.90
1:A:144:VAL:HG21	1:A:343:THR:HB	1.53	0.90
1:A:120:ARG:NH1	1:A:452:THR:CG2	2.34	0.90
1:A:120:ARG:HH12	1:A:452:THR:HG23	1.33	0.90
1:A:430:LEU:HD13	1:B:219:PHE:HD2	1.34	0.89
1:A:119:GLN:O	1:A:120:ARG:HD2	1.72	0.89
1:A:457:GLU:HG3	1:B:18:ARG:NH1	1.86	0.89
3:F:101:THR:O	3:F:101:THR:HG22	1.69	0.88
2:E:17:SER:HB2	2:E:83:ILE:O	1.74	0.87
3:D:136:ASN:HB3	3:D:137:ASN:ND2	1.90	0.86
2:C:17:SER:HB2	2:C:83:ILE:O	1.75	0.86
1:B:127:VAL:HB	1:B:157:ASN:ND2	1.91	0.86
1:A:419:TYR:HE1	1:A:422:ILE:HD12	1.38	0.86
1:A:430:LEU:HD13	1:B:219:PHE:CD2	2.10	0.86
3:F:54:THR:HG22	3:F:55:SER:H	1.40	0.86
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.10	0.86
1:B:362:ALA:O	1:B:366:VAL:HG23	1.74	0.86
2:C:100:TYR:HD2	2:C:101:TYR:N	1.74	0.85
1:B:109:ILE:CD1	4:B:474:BR:BR	2.77	0.85
1:A:120:ARG:NH1	1:A:452:THR:HG23	1.90	0.85
1:A:381:GLN:NE2	1:A:381:GLN:H	1.73	0.84
2:C:162:TRP:HD1	2:C:171:VAL:HG11	1.43	0.84
3:F:121:SER:HA	3:F:124:LEU:HD12	1.58	0.84
3:F:4:LEU:HD22	3:F:23:CYS:SG	2.18	0.83
1:A:227:ILE:HD13	1:B:423:LEU:HD21	1.59	0.83
1:A:32:PRO:HG2	1:A:35:ILE:HD13	1.59	0.83
1:A:423:LEU:O	1:A:427:ILE:HD13	1.77	0.83
1:A:430:LEU:CD1	1:B:219:PHE:HD2	1.90	0.83
3:F:95:GLN:OE1	3:F:95:GLN:N	2.11	0.83
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.43	0.83
2:C:17:SER:HB3	2:C:84:SER:HA	1.61	0.82
2:E:38:ARG:HD3	2:E:94:TYR:CE1	2.15	0.82
1:B:381:GLN:H	1:B:381:GLN:NE2	1.77	0.82
3:F:190:SER:HA	3:F:209:ASN:OD1	1.78	0.81
2:E:91:THR:OG1	2:E:119:VAL:HG23	1.79	0.81
1:B:148:GLU:H	1:B:148:GLU:CD	1.80	0.81
1:A:207:GLN:HG2	1:B:28:ARG:NE	1.96	0.81
1:A:22:ILE:HD12	1:B:453:LEU:HB3	1.64	0.80
1:B:154:ILE:O	1:B:158:ILE:HG12	1.79	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:ILE:CD1	1:B:426:ILE:HG22	2.07	0.80
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.64	0.80
1:A:287:ASN:ND2	1:A:290:LYS:H	1.79	0.80
1:A:231:ILE:HG22	1:A:232:PHE:HD1	1.44	0.80
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.17	0.80
1:A:426:ILE:HG21	1:B:223:ILE:HD11	1.64	0.79
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.17	0.79
3:D:7:SER:HB2	3:D:22:THR:HB	1.64	0.79
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.65	0.79
1:B:198:LEU:HD13	1:B:201:ILE:HD11	1.65	0.79
2:C:129:VAL:HG21	2:C:214:VAL:CG1	2.12	0.79
3:F:31:TYR:HA	3:F:50:THR:OG1	1.81	0.79
1:A:419:TYR:CE1	1:A:422:ILE:HD12	2.17	0.79
1:A:200:ILE:HA	1:A:204:MET:HB2	1.63	0.79
1:B:131:LYS:HE2	1:B:153:GLN:HE22	1.45	0.78
3:F:189:ASN:HD21	3:F:210:ARG:HB2	1.48	0.78
1:A:207:GLN:HG2	1:B:28:ARG:HE	1.48	0.78
1:A:65:MET:HA	1:A:65:MET:CE	2.13	0.78
1:B:175:HIS:HB3	1:B:213:ILE:HD12	1.64	0.78
1:B:131:LYS:CE	1:B:153:GLN:NE2	2.36	0.78
3:D:143:ILE:HD12	3:D:197:HIS:HB2	1.66	0.77
1:A:231:ILE:HG22	1:A:232:PHE:CE1	2.18	0.77
1:B:32:PRO:HB2	1:B:35:ILE:HD13	1.66	0.77
2:C:172:HIS:CE1	3:D:173:SER:HG	2.03	0.77
3:D:95:GLN:H	3:D:95:GLN:CD	1.86	0.77
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.65	0.77
1:A:37:PHE:HD2	1:A:38:MET:CE	1.98	0.76
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.57	0.76
3:F:13:ALA:HB1	3:F:17:ASP:OD1	1.86	0.76
1:B:287:ASN:HD22	1:B:290:LYS:H	1.28	0.76
1:A:87:ALA:O	1:A:91:MET:HG3	1.85	0.76
1:A:107:SER:OG	1:A:109:ILE:HD13	1.86	0.76
2:C:162:TRP:CD1	2:C:171:VAL:CG1	2.69	0.76
2:C:172:HIS:CE1	3:D:173:SER:OG	2.39	0.76
1:B:277:GLN:HE22	1:B:448:ILE:HD11	1.51	0.75
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.67	0.75
2:E:17:SER:HB2	2:E:84:SER:HA	1.67	0.75
2:E:135:GLY:HA2	2:E:221:ARG:CD	2.17	0.75
1:A:148:GLU:CG	1:A:190:PHE:CZ	2.70	0.74
2:C:51:ILE:HD13	2:C:52:ASN:N	2.02	0.74
1:A:422:ILE:HD11	1:B:194:LEU:HG	1.68	0.74
3:F:49:ASP:O	3:F:51:SER:N	2.21	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.70	0.74
1:B:197:ILE:HG13	1:B:219:PHE:CE1	2.22	0.74
3:F:184:GLU:HA	3:F:187:ARG:NH1	2.02	0.73
1:A:227:ILE:CD1	1:B:423:LEU:HD21	2.18	0.73
1:B:422:ILE:HA	1:B:425:MET:HE2	1.69	0.73
2:C:30:SER:O	2:C:32:TYR:N	2.21	0.72
2:C:150:VAL:CG1	2:C:205:VAL:HG11	2.12	0.72
1:B:257:ILE:HG22	1:B:371:PHE:CE1	2.24	0.72
2:E:30:SER:O	2:E:31:ARG:HB2	1.89	0.72
1:B:201:ILE:HD12	1:B:202:GLU:N	2.04	0.72
1:B:184:ALA:HB1	1:B:225:SER:HB2	1.70	0.72
1:B:451:ARG:HH11	1:B:451:ARG:HG3	1.53	0.72
1:A:381:GLN:HE21	1:A:381:GLN:H	1.35	0.72
2:C:67:LYS:NZ	2:C:85:LYS:O	2.23	0.72
2:C:162:TRP:HD1	2:C:171:VAL:CG1	2.03	0.71
2:E:181:ALA:O	2:E:182:LEU:HD23	1.90	0.71
1:B:451:ARG:CG	1:B:451:ARG:HH11	2.02	0.71
2:E:48:ILE:HD12	2:E:68:PHE:CZ	2.24	0.71
2:C:17:SER:CB	2:C:84:SER:HA	2.21	0.71
3:F:7:SER:CB	3:F:22:THR:HB	2.17	0.71
1:A:148:GLU:HG2	1:A:190:PHE:CZ	2.26	0.71
2:E:51:ILE:CD1	2:E:55:SER:HA	2.16	0.71
1:B:257:ILE:HG22	1:B:371:PHE:CZ	2.25	0.71
3:D:7:SER:CB	3:D:8:PRO:CD	2.49	0.71
3:F:148:LYS:HB2	3:F:192:THR:OG1	1.91	0.71
3:F:33:HIS:CE1	3:F:49:ASP:H	2.08	0.71
3:F:107:ARG:HG3	3:F:139:TYR:CD1	2.25	0.71
3:F:129:ALA:O	3:F:179:THR:HA	1.90	0.71
2:E:38:ARG:HB3	2:E:94:TYR:CD1	2.25	0.71
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.21	0.70
2:C:129:VAL:HG13	2:C:150:VAL:HG13	1.72	0.70
1:B:241:VAL:HG21	1:B:416:THR:HG22	1.73	0.70
1:A:294:MET:O	1:A:298:ILE:HG13	1.92	0.70
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.73	0.70
2:C:163:ASN:HB2	2:C:167:LEU:HD13	1.74	0.70
2:E:94:TYR:CD2	2:E:117:VAL:CG2	2.75	0.69
1:A:22:ILE:CD1	1:B:453:LEU:HB3	2.22	0.69
3:F:112:PRO:HG3	3:F:143:ILE:HD11	1.73	0.69
2:E:130:TYR:HE2	2:E:151:LYS:HG2	1.57	0.69
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.73	0.69
3:F:49:ASP:CB	3:F:52:LYS:HE3	2.23	0.68
1:B:159:GLY:O	1:B:162:VAL:HG22	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:77:MET:HG3	3:F:78:GLU:N	2.08	0.68
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.74	0.68
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.75	0.68
1:A:241:VAL:CG1	1:A:324:THR:HG21	2.19	0.68
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.28	0.68
3:D:187:ARG:HG3	3:D:188:HIS:CD2	2.29	0.68
2:C:30:SER:C	2:C:32:TYR:H	1.97	0.68
1:A:158:ILE:O	1:A:162:VAL:HG13	1.93	0.68
2:E:38:ARG:NH1	2:E:94:TYR:OH	2.25	0.68
3:D:136:ASN:HB3	3:D:137:ASN:HD22	1.56	0.68
2:C:162:TRP:CD1	2:C:171:VAL:HG11	2.28	0.68
2:E:51:ILE:HD13	2:E:52:ASN:N	2.09	0.67
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.29	0.67
2:E:39:GLN:O	2:E:92:ALA:HB1	1.94	0.67
3:F:4:LEU:HD23	3:F:25:ALA:HB2	1.76	0.67
1:A:183:ALA:HB2	1:A:200:ILE:HD13	1.76	0.67
2:E:163:ASN:HB2	2:E:167:LEU:HD13	1.77	0.67
1:A:220:ILE:CG1	1:B:430:LEU:HD21	2.25	0.67
1:B:86:SER:HB3	1:B:299:GLY:O	1.95	0.67
1:A:357:PHE:CE1	1:A:402:ILE:HD13	2.28	0.67
1:A:143:MET:HA	1:A:302:CYS:SG	2.34	0.67
1:B:127:VAL:HB	1:B:157:ASN:HD22	1.59	0.67
3:F:101:THR:O	3:F:101:THR:CG2	2.42	0.67
1:A:414:GLU:HG2	1:B:419:TYR:OH	1.95	0.67
1:B:175:HIS:HB3	1:B:213:ILE:CD1	2.25	0.67
3:F:30:SER:HA	3:F:70:TYR:OH	1.95	0.67
1:A:42:VAL:O	1:A:46:VAL:HG23	1.94	0.67
1:A:332:MET:CE	1:A:336:ILE:HD11	2.25	0.67
1:B:38:MET:O	1:B:42:VAL:HG23	1.96	0.66
2:E:58:ILE:CG2	2:E:58:ILE:O	2.41	0.66
3:F:7:SER:HB2	3:F:22:THR:CB	2.20	0.66
3:D:134:PHE:HB3	3:D:136:ASN:HD21	1.61	0.66
3:D:116:ILE:HD11	3:D:131:VAL:CG1	2.25	0.66
3:D:116:ILE:HD11	3:D:131:VAL:HG13	1.78	0.66
3:D:150:ASP:OD2	3:D:190:SER:N	2.27	0.66
3:D:168:LYS:O	3:D:169:ASP:HB3	1.96	0.66
1:B:203:GLU:OE2	1:B:445:LEU:HD23	1.95	0.66
3:F:27:SER:O	3:F:68:THR:HG22	1.95	0.66
3:F:185:TYR:HA	3:F:191:TYR:OH	1.96	0.66
1:A:260:ILE:O	1:A:264:ILE:HG23	1.96	0.66
1:B:176:THR:O	1:B:180:THR:HG23	1.96	0.66
1:A:206:PRO:HG2	1:A:211:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:ARG:HH11	1:A:230:ARG:HG2	1.61	0.66
1:B:197:ILE:HD13	1:B:218:VAL:HG12	1.78	0.66
2:E:94:TYR:HD2	2:E:117:VAL:CG2	2.09	0.66
2:E:17:SER:HB3	2:E:84:SER:CA	2.19	0.65
1:A:277:GLN:HE22	1:A:448:ILE:HD11	1.62	0.65
1:B:391:ILE:CD1	1:B:416:THR:HG21	2.25	0.65
2:C:162:TRP:CD1	2:C:171:VAL:HG13	2.30	0.65
3:D:77:MET:HE3	3:D:78:GLU:O	1.97	0.65
1:A:244:LEU:HG	1:A:391:ILE:CD1	2.27	0.65
2:E:130:TYR:CE2	2:E:151:LYS:HG2	2.32	0.65
3:F:191:TYR:O	3:F:207:SER:CB	2.38	0.65
1:A:451:ARG:HH11	1:A:451:ARG:CG	2.08	0.65
1:A:410:ILE:HD11	1:B:194:LEU:HD13	1.79	0.64
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.33	0.64
3:F:150:ASP:OD1	3:F:188:HIS:HB3	1.98	0.64
3:F:192:THR:HA	3:F:207:SER:HB3	1.79	0.64
1:A:244:LEU:HG	1:A:391:ILE:HD11	1.79	0.64
1:B:59:TRP:O	1:B:63:GLN:HG2	1.97	0.64
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.28	0.64
3:F:145:VAL:HA	3:F:194:GLU:O	1.97	0.64
3:F:7:SER:HB3	3:F:8:PRO:HD2	1.78	0.64
1:B:408:GLY:O	1:B:412:VAL:HG23	1.98	0.64
1:A:457:GLU:HG3	1:B:18:ARG:HH11	1.61	0.64
1:B:107:SER:OG	4:B:474:BR:BR	2.67	0.64
1:A:88:VAL:HA	1:A:91:MET:HE2	1.79	0.64
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.63	0.64
1:A:184:ALA:HB1	1:A:225:SER:HB3	1.80	0.64
3:D:116:ILE:HD12	3:D:208:PHE:CD2	2.33	0.63
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.32	0.63
1:B:54:ASP:OD1	1:B:147:ARG:NH2	2.26	0.63
1:A:148:GLU:HG2	1:A:190:PHE:HZ	1.63	0.63
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.33	0.63
1:B:381:GLN:HG2	1:B:382:TYR:N	2.12	0.63
1:B:197:ILE:HG13	1:B:219:PHE:HE1	1.63	0.63
1:A:176:THR:O	1:A:180:THR:HG23	1.98	0.63
1:B:53:PHE:O	1:B:57:VAL:HG23	1.97	0.63
1:B:148:GLU:HG3	1:B:190:PHE:CZ	2.33	0.63
1:A:194:LEU:HD11	1:B:422:ILE:HD11	1.81	0.63
2:E:137:ALA:O	2:E:139:ALA:N	2.31	0.63
1:B:287:ASN:HD22	1:B:290:LYS:N	1.97	0.63
3:F:140:PRO:HD2	3:F:198:LYS:HD2	1.81	0.63
1:A:241:VAL:HG11	1:A:324:THR:CG2	2.22	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:134:PRO:O	2:C:135:GLY:O	2.17	0.62
3:F:30:SER:H	3:F:91:SER:CB	2.12	0.62
3:F:57:VAL:O	3:F:57:VAL:HG12	1.98	0.62
2:E:67:LYS:NZ	2:E:85:LYS:O	2.32	0.62
1:A:165:ILE:HG22	1:A:166:PHE:CD2	2.34	0.62
3:F:117:PHE:HB2	3:F:132:VAL:HB	1.82	0.62
3:F:90:TRP:CD2	3:F:95:GLN:HB3	2.35	0.62
1:A:257:ILE:HD12	1:A:257:ILE:H	1.65	0.62
1:A:148:GLU:H	1:A:148:GLU:CD	2.02	0.62
3:F:77:MET:HE1	3:F:103:LEU:HD21	1.82	0.62
3:D:50:THR:HG22	3:D:64:SER:HA	1.81	0.61
1:B:98:ARG:HB3	1:B:288:ILE:HG13	1.81	0.61
3:F:32:ILE:O	3:F:50:THR:HA	2.00	0.61
1:A:457:GLU:HG3	1:B:18:ARG:HH12	1.62	0.61
1:A:28:ARG:HE	1:B:207:GLN:HG2	1.65	0.61
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.00	0.61
3:F:83:ALA:HB3	3:F:85:TYR:CE1	2.36	0.61
2:C:122:ALA:HB3	2:C:154:PHE:CE2	2.36	0.61
2:E:38:ARG:HB3	2:E:94:TYR:CE1	2.34	0.61
1:A:17:ARG:HE	1:A:18:ARG:N	1.99	0.61
1:B:402:ILE:HD12	1:B:402:ILE:O	2.01	0.61
2:C:199:GLU:HG2	2:C:200:THR:N	2.14	0.61
3:D:149:ILE:HD12	3:D:154:ARG:HB2	1.83	0.61
3:D:154:ARG:HG3	3:D:155:GLN:H	1.65	0.61
2:E:47:TRP:CE2	3:F:95:GLN:NE2	2.68	0.61
3:D:188:HIS:O	3:D:210:ARG:HD3	2.01	0.60
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.82	0.60
1:A:270:ASN:HD22	1:A:270:ASN:N	1.99	0.60
2:E:59:ASN:OD1	2:E:59:ASN:N	2.32	0.60
1:B:77:LEU:O	1:B:81:VAL:HG13	2.00	0.60
1:B:357:PHE:CD2	4:B:474:BR:BR	3.09	0.60
1:B:281:HIS:HA	1:B:284:HIS:HE1	1.67	0.60
2:E:2:VAL:O	2:E:3:ARG:CB	2.40	0.60
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.30	0.60
2:C:129:VAL:HG11	2:C:205:VAL:HG21	1.83	0.60
3:F:116:ILE:HG22	3:F:206:LYS:HE2	1.83	0.60
2:E:162:TRP:CE3	2:E:203:CYS:HB3	2.36	0.60
3:D:197:HIS:O	3:D:199:THR:N	2.33	0.60
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.82	0.60
1:A:264:ILE:HG12	1:A:265:PHE:N	2.15	0.60
3:D:6:GLN:HG3	3:D:100:GLY:N	2.17	0.60
1:A:381:GLN:N	1:A:381:GLN:HE21	1.99	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:269:PHE:O	1:B:273:VAL:HG12	2.02	0.60
1:A:459:GLU:O	1:A:460:GLN:NE2	2.34	0.60
3:F:150:ASP:CA	3:F:190:SER:HB3	2.26	0.60
1:A:148:GLU:HG3	1:A:190:PHE:CZ	2.35	0.60
1:B:402:ILE:HD13	1:B:445:LEU:HD22	1.83	0.60
1:A:120:ARG:HH11	1:A:452:THR:CG2	2.14	0.60
1:A:219:PHE:HD2	1:B:430:LEU:HD13	1.66	0.60
2:E:94:TYR:CD2	2:E:117:VAL:HG21	2.37	0.60
3:D:77:MET:HG2	3:D:78:GLU:H	1.67	0.60
1:A:231:ILE:HD13	1:B:249:LEU:CD1	2.32	0.60
3:F:29:VAL:HG11	3:F:89:GLN:HG2	1.83	0.60
3:F:61:PHE:HE2	3:F:85:TYR:HE2	1.48	0.59
1:A:36:LEU:HD13	1:B:434:LEU:HD21	1.83	0.59
3:F:54:THR:HG22	3:F:55:SER:N	2.14	0.59
1:A:414:GLU:HG2	1:B:419:TYR:CZ	2.37	0.59
1:B:107:SER:N	4:B:475:BR:BR	2.89	0.59
3:F:21:MET:HB3	3:F:101:THR:HG21	1.84	0.59
2:C:174:PHE:HD2	2:C:186:SER:O	1.85	0.59
3:D:146:LYS:HE3	3:D:153:GLU:CD	2.23	0.59
1:B:197:ILE:CD1	1:B:218:VAL:HG12	2.32	0.59
1:A:427:ILE:N	1:A:427:ILE:CD1	2.66	0.59
3:F:169:ASP:OD1	3:F:171:THR:HG23	2.02	0.59
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.35	0.59
2:C:42:GLY:O	2:C:43:LYS:CB	2.50	0.59
1:A:238:LEU:C	1:A:239:ILE:HD12	2.23	0.59
1:A:451:ARG:HG3	1:A:451:ARG:NH1	2.16	0.59
1:A:65:MET:HE3	1:A:65:MET:HA	1.83	0.59
3:D:181:THR:OG1	3:D:184:GLU:HB3	2.02	0.59
3:D:158:VAL:HA	3:D:177:THR:O	2.03	0.59
2:C:162:TRP:CH2	2:C:203:CYS:HB3	2.37	0.59
2:C:42:GLY:O	2:C:43:LYS:HB2	2.02	0.58
2:C:129:VAL:CG2	2:C:214:VAL:HG11	2.33	0.58
3:F:77:MET:HE1	3:F:103:LEU:CD2	2.33	0.58
3:F:19:VAL:HB	3:F:74:ILE:HD13	1.86	0.58
2:E:61:THR:O	2:E:63:SER:N	2.35	0.58
3:F:189:ASN:ND2	3:F:210:ARG:HB2	2.18	0.58
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.22	0.58
2:E:69:ILE:HD13	2:E:82:GLN:HB3	1.86	0.58
3:F:123:GLN:OE1	3:F:130:SER:HB2	2.04	0.58
1:B:175:HIS:CB	1:B:213:ILE:HD12	2.33	0.58
1:A:276:MET:HB3	1:A:349:SER:OG	2.04	0.58
3:D:162:TRP:H	3:D:162:TRP:HE3	1.52	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:PHE:CZ	1:B:426:ILE:HD12	2.38	0.57
3:D:6:GLN:HG3	3:D:100:GLY:H	1.69	0.57
1:A:335:PHE:CD1	1:A:336:ILE:HD12	2.39	0.57
1:B:381:GLN:N	1:B:381:GLN:HE21	1.90	0.57
2:E:152:GLY:C	2:E:182:LEU:HD13	2.24	0.57
1:A:123:ARG:NE	1:A:126:ARG:HD2	2.09	0.57
3:D:134:PHE:HB3	3:D:136:ASN:ND2	2.18	0.57
1:A:276:MET:HB3	1:A:349:SER:CB	2.34	0.57
3:D:205:VAL:HG23	3:D:206:LYS:N	2.19	0.57
2:C:52:ASN:HB2	2:C:53:PRO:HD2	1.84	0.57
1:B:241:VAL:CG2	1:B:416:THR:HG22	2.35	0.57
3:F:74:ILE:HD12	3:F:74:ILE:H	1.68	0.57
1:A:57:VAL:HG11	1:A:139:LEU:HB3	1.86	0.57
3:D:154:ARG:HG3	3:D:155:GLN:N	2.19	0.57
3:F:89:GLN:O	3:F:95:GLN:HB2	2.04	0.57
1:B:248:PRO:HB3	2:E:104:GLY:HA3	1.85	0.57
2:E:32:TYR:O	2:E:72:ARG:NH2	2.35	0.56
2:E:69:ILE:HD12	2:E:82:GLN:O	2.05	0.56
1:B:262:PHE:HZ	1:B:364:GLY:HA2	1.68	0.56
1:A:51:VAL:CG1	1:A:232:PHE:HD2	2.07	0.56
2:C:47:TRP:CE2	3:D:95:GLN:NE2	2.74	0.56
2:C:100:TYR:CD2	2:C:101:TYR:N	2.57	0.56
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.87	0.56
1:B:148:GLU:N	1:B:148:GLU:CD	2.55	0.56
2:E:51:ILE:CD1	2:E:52:ASN:O	2.54	0.56
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.21	0.56
3:D:136:ASN:HD22	3:D:136:ASN:N	2.04	0.56
1:B:379:PHE:HB3	1:B:382:TYR:HD1	1.71	0.56
3:D:31:TYR:HA	3:D:50:THR:OG1	2.05	0.56
3:D:127:GLY:HA2	3:D:182:LYS:HB2	1.86	0.56
1:B:379:PHE:HB3	1:B:382:TYR:CD1	2.41	0.56
2:E:130:TYR:HD2	2:E:149:LEU:HD23	1.70	0.56
3:F:41:THR:HG23	3:F:42:SER:O	2.04	0.56
1:A:86:SER:HB3	1:A:299:GLY:O	2.06	0.56
2:E:221:ARG:NH2	3:F:118:PRO:HB2	2.21	0.56
1:B:305:LEU:HA	1:B:308:VAL:CG2	2.34	0.56
2:C:51:ILE:HG12	2:C:58:ILE:HG12	1.87	0.56
1:A:257:ILE:HD12	1:A:257:ILE:N	2.21	0.56
3:F:119:PRO:HB2	3:F:124:LEU:HD21	1.87	0.56
2:E:152:GLY:CA	2:E:182:LEU:HD13	2.36	0.56
2:E:52:ASN:ND2	2:E:57:THR:HB	2.21	0.55
3:F:46:TRP:C	3:F:47:ILE:HD12	2.26	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:104:ALA:HB1	1:B:131:LYS:HD3	1.88	0.55
3:F:21:MET:CE	3:F:74:ILE:HD11	2.36	0.55
1:A:459:GLU:C	1:A:460:GLN:HE21	2.09	0.55
2:C:177:VAL:O	2:C:183:TYR:HA	2.06	0.55
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.88	0.55
3:F:6:GLN:HG3	3:F:99:GLY:H	1.71	0.55
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.89	0.55
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.35	0.55
3:F:30:SER:N	3:F:91:SER:OG	2.34	0.55
1:A:437:GLN:HE21	1:B:216:LYS:NZ	2.04	0.55
1:A:31:THR:HG21	1:A:214:SER:HB2	1.89	0.55
1:B:266:GLY:HA3	1:B:400:ALA:HB1	1.89	0.55
3:F:11:MET:CE	3:F:19:VAL:HG13	2.36	0.55
3:F:77:MET:CG	3:F:78:GLU:N	2.70	0.55
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.88	0.55
3:D:191:TYR:O	3:D:207:SER:HB2	2.06	0.55
1:B:287:ASN:ND2	1:B:290:LYS:N	2.44	0.55
2:C:129:VAL:HG21	2:C:214:VAL:HG11	1.87	0.55
3:D:149:ILE:HG23	3:D:191:TYR:CE2	2.41	0.55
3:F:197:HIS:O	3:F:199:THR:N	2.40	0.54
3:F:9:ALA:C	3:F:10:ILE:HD12	2.27	0.54
2:C:153:TYR:CE2	2:C:183:TYR:HB3	2.41	0.54
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.23	0.54
1:B:262:PHE:CZ	1:B:364:GLY:HA2	2.42	0.54
1:A:216:LYS:NZ	1:B:433:THR:HG22	2.23	0.54
3:D:145:VAL:HG11	3:D:174:MET:HE1	1.88	0.54
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.88	0.54
2:C:204:ASN:HB3	2:C:215:ASP:OD1	2.07	0.54
2:C:153:TYR:CE1	2:C:158:VAL:HG13	2.42	0.54
2:E:36:TRP:HD1	2:E:70:ILE:HG13	1.72	0.54
1:B:327:ASN:N	1:B:327:ASN:HD22	2.06	0.54
3:D:131:VAL:HG12	3:D:147:TRP:CH2	2.43	0.54
2:C:94:TYR:O	2:C:114:GLY:HA2	2.08	0.54
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.89	0.54
3:D:187:ARG:O	3:D:188:HIS:CG	2.61	0.54
3:F:32:ILE:HG22	3:F:89:GLN:HB3	1.90	0.54
3:D:17:ASP:H	3:D:76:THR:HA	1.73	0.54
2:E:36:TRP:CG	2:E:81:LEU:HD22	2.42	0.54
1:B:197:ILE:HD13	1:B:222:VAL:HG21	1.90	0.54
3:F:14:ALA:O	3:F:17:ASP:HB2	2.08	0.54
1:B:402:ILE:HD13	1:B:445:LEU:CD2	2.37	0.54
3:F:7:SER:O	3:F:9:ALA:N	2.41	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:150:VAL:HG11	2:C:205:VAL:CG1	2.18	0.53
1:B:200:ILE:HA	1:B:204:MET:HB2	1.89	0.53
1:B:32:PRO:CB	1:B:35:ILE:HD13	2.36	0.53
1:B:32:PRO:HG2	1:B:35:ILE:HD13	1.89	0.53
1:A:37:PHE:HD2	1:A:38:MET:HE1	1.72	0.53
1:A:184:ALA:HB1	1:A:225:SER:CB	2.38	0.53
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.89	0.53
2:C:89:GLU:OE2	2:C:89:GLU:N	2.42	0.53
3:D:82:ALA:HB2	3:D:105:ILE:CD1	2.18	0.53
1:B:206:PRO:CG	1:B:211:THR:OG1	2.48	0.53
3:F:74:ILE:HD12	3:F:74:ILE:N	2.23	0.53
1:B:316:GLY:O	1:B:320:ILE:HD12	2.08	0.53
1:A:341:VAL:O	1:A:345:LEU:HG	2.07	0.53
1:A:287:ASN:HD21	1:A:290:LYS:H	1.54	0.53
1:B:202:GLU:OE1	1:B:407:THR:HB	2.08	0.53
2:C:130:TYR:HB2	2:C:149:LEU:HB3	1.91	0.53
3:D:192:THR:HA	3:D:207:SER:CB	2.37	0.53
1:B:197:ILE:HG13	1:B:219:PHE:CD1	2.43	0.53
1:B:91:MET:HG2	1:B:292:VAL:O	2.09	0.53
3:D:148:LYS:HG3	3:D:153:GLU:HA	1.91	0.53
1:B:127:VAL:O	1:B:128:LEU:C	2.47	0.53
3:F:80:GLU:HA	3:F:167:SER:O	2.09	0.53
1:A:248:PRO:O	1:A:251:THR:HB	2.09	0.53
3:F:139:TYR:CD2	3:F:140:PRO:HA	2.43	0.53
1:A:160:ARG:O	1:A:163:LEU:HB3	2.09	0.53
3:D:32:ILE:H	3:D:32:ILE:CD1	2.22	0.53
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.44	0.53
2:E:76:LYS:O	2:E:77:ASP:HB2	2.09	0.53
2:C:129:VAL:CG2	2:C:214:VAL:CG1	2.87	0.53
3:F:49:ASP:O	3:F:50:THR:C	2.45	0.53
1:B:165:ILE:O	1:B:165:ILE:HG22	2.09	0.53
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.90	0.53
2:E:94:TYR:CE2	2:E:117:VAL:HG21	2.43	0.53
2:E:86:VAL:HG13	2:E:90:ASP:HB2	1.91	0.53
3:F:6:GLN:NE2	3:F:98:GLY:HA3	2.24	0.52
2:C:163:ASN:HD21	2:C:201:VAL:HA	1.74	0.52
1:A:277:GLN:HE22	1:A:448:ILE:CD1	2.21	0.52
3:F:93:HIS:HA	3:F:94:PRO:C	2.30	0.52
1:B:95:PHE:O	1:B:97:VAL:N	2.42	0.52
3:D:131:VAL:HG12	3:D:147:TRP:HH2	1.74	0.52
1:A:400:ALA:HB2	1:A:432:ALA:HB1	1.90	0.52
1:B:92:PHE:C	1:B:92:PHE:CD1	2.83	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.89	0.52
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.90	0.52
1:A:57:VAL:HG23	1:A:136:LEU:HD12	1.92	0.52
1:B:321:PRO:HB2	1:B:322:ILE:HD12	1.92	0.52
3:D:95:GLN:CA	3:D:95:GLN:OE1	2.51	0.52
2:E:30:SER:O	2:E:31:ARG:CB	2.54	0.52
3:D:66:SER:HA	3:D:70:TYR:CZ	2.43	0.52
1:A:62:ASN:OD1	1:A:63:GLN:NE2	2.42	0.52
1:B:451:ARG:CB	1:B:451:ARG:HH11	2.23	0.52
1:A:192:ALA:HB1	1:A:414:GLU:OE2	2.09	0.52
1:A:284:HIS:CE1	1:A:291:TRP:CD2	2.97	0.52
1:A:104:ALA:HB2	1:A:127:VAL:HG22	1.91	0.52
2:E:70:ILE:N	2:E:70:ILE:CD1	2.73	0.52
1:A:62:ASN:O	1:A:65:MET:HB3	2.10	0.52
2:E:47:TRP:CD2	3:F:95:GLN:NE2	2.78	0.52
1:B:357:PHE:CE1	1:B:398:LEU:HD21	2.45	0.52
3:D:32:ILE:CD1	3:D:50:THR:HG23	2.40	0.52
1:B:327:ASN:ND2	1:B:327:ASN:N	2.58	0.52
3:D:7:SER:HB2	3:D:22:THR:CB	2.37	0.52
3:F:77:MET:HE1	3:F:103:LEU:CD1	2.40	0.52
3:D:9:ALA:O	3:D:10:ILE:HD13	2.10	0.52
1:A:231:ILE:CG2	1:A:232:PHE:CE1	2.93	0.51
1:B:197:ILE:CD1	1:B:222:VAL:HG21	2.40	0.51
2:E:4:LEU:HB3	2:E:22:CYS:SG	2.49	0.51
2:E:135:GLY:HA2	2:E:221:ARG:HD2	1.91	0.51
3:F:189:ASN:HD21	3:F:210:ARG:CB	2.21	0.51
2:E:94:TYR:CD2	2:E:117:VAL:HG23	2.45	0.51
1:B:36:LEU:HD22	1:B:220:ILE:HD11	1.92	0.51
1:A:199:PHE:HA	1:A:407:THR:OG1	2.10	0.51
1:A:114:GLY:HA3	1:A:120:ARG:HG2	1.93	0.51
2:E:30:SER:C	2:E:32:TYR:H	2.14	0.51
1:A:31:THR:HG21	1:A:214:SER:CB	2.40	0.51
3:D:7:SER:HB2	3:D:22:THR:N	2.25	0.51
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.76	0.51
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.45	0.51
2:E:38:ARG:HD3	2:E:94:TYR:HE1	1.74	0.51
1:A:17:ARG:HG3	1:A:18:ARG:H	1.76	0.51
1:B:71:THR:HG21	1:B:81:VAL:HG11	1.93	0.51
1:B:191:ASN:HD21	1:B:230:ARG:NH1	2.09	0.51
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.93	0.51
1:A:165:ILE:HG22	1:A:166:PHE:HD2	1.74	0.51
1:A:253:TRP:O	1:A:257:ILE:CD1	2.58	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:94:TYR:CE2	2:E:117:VAL:CG2	2.93	0.51
3:F:189:ASN:ND2	3:F:210:ARG:H	2.08	0.51
2:E:193:SER:O	2:E:196:TRP:O	2.29	0.51
1:B:287:ASN:O	1:B:289:THR:N	2.44	0.51
2:E:92:ALA:O	2:E:116:THR:HA	2.11	0.51
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.46	0.51
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.46	0.51
3:D:61:PHE:CE2	3:D:74:ILE:HG12	2.46	0.51
2:E:51:ILE:HD13	2:E:52:ASN:O	2.11	0.51
1:A:264:ILE:HG22	1:A:435:LEU:HD12	1.93	0.51
1:B:322:ILE:HD12	1:B:322:ILE:N	2.26	0.51
1:B:309:ALA:O	1:B:311:ALA:N	2.44	0.51
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.44	0.51
1:A:399:ALA:O	1:A:403:ARG:HA	2.11	0.50
1:A:107:SER:HG	1:A:109:ILE:HD13	1.77	0.50
3:F:107:ARG:HG3	3:F:139:TYR:CE1	2.45	0.50
3:F:85:TYR:CD1	3:F:85:TYR:N	2.78	0.50
1:A:94:TYR:O	1:A:98:ARG:HG2	2.12	0.50
1:B:322:ILE:H	1:B:322:ILE:HD12	1.76	0.50
1:B:127:VAL:HB	1:B:157:ASN:HD21	1.73	0.50
1:A:148:GLU:CG	1:A:190:PHE:HZ	2.20	0.50
2:E:91:THR:HA	2:E:117:VAL:O	2.12	0.50
3:D:162:TRP:N	3:D:162:TRP:CE3	2.79	0.50
2:E:41:PRO:O	2:E:43:LYS:HG3	2.10	0.50
2:C:47:TRP:CD2	3:D:95:GLN:NE2	2.80	0.50
3:F:77:MET:HE1	3:F:103:LEU:HD11	1.92	0.50
1:A:83:PHE:C	1:A:83:PHE:CD1	2.84	0.50
3:D:143:ILE:HD12	3:D:197:HIS:CB	2.40	0.50
3:F:138:PHE:CG	3:F:143:ILE:HD12	2.47	0.50
1:A:145:LEU:HD21	1:A:347:CYS:HB3	1.94	0.50
1:B:148:GLU:O	1:B:149:GLY:C	2.47	0.50
3:D:19:VAL:O	3:D:73:THR:HA	2.11	0.50
3:F:192:THR:HA	3:F:207:SER:CB	2.41	0.50
1:A:402:ILE:HG23	1:A:445:LEU:HD22	1.94	0.50
3:F:86:TYR:CD1	3:F:86:TYR:N	2.79	0.49
1:B:42:VAL:O	1:B:46:VAL:HG23	2.12	0.49
1:B:176:THR:O	1:B:180:THR:CG2	2.59	0.49
2:C:38:ARG:NH1	2:C:90:ASP:HA	2.27	0.49
3:D:32:ILE:H	3:D:32:ILE:HD12	1.77	0.49
1:A:202:GLU:OE1	1:A:404:ALA:HB1	2.12	0.49
1:B:311:ALA:HB3	1:B:336:ILE:HD11	1.94	0.49
1:B:93:GLY:O	1:B:97:VAL:CG2	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:451:ARG:NH1	1:B:451:ARG:HG3	2.20	0.49
1:A:216:LYS:HZ1	1:B:433:THR:HG22	1.75	0.49
1:B:399:ALA:O	1:B:403:ARG:HA	2.13	0.49
2:C:101:TYR:HB2	2:C:104:GLY:HA2	1.94	0.49
1:A:31:THR:CG2	1:A:214:SER:HB2	2.42	0.49
3:D:46:TRP:HB3	3:D:47:ILE:HD12	1.93	0.49
2:E:70:ILE:N	2:E:70:ILE:HD12	2.27	0.49
3:F:138:PHE:CD1	3:F:143:ILE:HD12	2.47	0.49
1:B:160:ARG:O	1:B:163:LEU:HB3	2.11	0.49
1:B:119:GLN:O	1:B:120:ARG:HD2	2.13	0.49
1:A:456:GLN:OE1	1:B:18:ARG:NH2	2.45	0.49
1:B:109:ILE:N	1:B:110:PRO:HD2	2.27	0.49
1:B:357:PHE:HD2	4:B:474:BR:BR	2.50	0.49
1:B:148:GLU:CG	1:B:190:PHE:CZ	2.96	0.49
1:A:284:HIS:CE1	1:A:291:TRP:CE3	3.01	0.49
2:C:6:GLU:HA	2:C:22:CYS:HA	1.95	0.49
1:B:200:ILE:HG22	1:B:201:ILE:N	2.28	0.49
2:E:151:LYS:NZ	2:E:151:LYS:HB2	2.28	0.49
1:B:42:VAL:HG21	1:B:177:LEU:HD22	1.95	0.49
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.31	0.49
1:B:348:PHE:HB2	1:B:356:ILE:HD13	1.95	0.49
2:C:129:VAL:HG21	2:C:214:VAL:HG12	1.90	0.49
2:C:52:ASN:CB	2:C:53:PRO:CD	2.91	0.49
1:A:241:VAL:CG1	1:A:324:THR:CG2	2.88	0.49
1:A:227:ILE:HD12	1:B:252:LEU:CD1	2.43	0.49
1:A:305:LEU:C	1:A:307:PHE:H	2.14	0.49
1:B:146:GLY:HA3	1:B:358:ALA:HB3	1.93	0.49
2:E:20:LEU:N	2:E:81:LEU:O	2.44	0.48
3:D:116:ILE:HD13	3:D:117:PHE:H	1.72	0.48
3:D:185:TYR:CD1	3:D:191:TYR:CE1	3.00	0.48
1:A:107:SER:OG	4:A:474:BR:BR	2.77	0.48
1:A:230:ARG:NH1	1:A:230:ARG:HG2	2.23	0.48
1:B:348:PHE:CB	1:B:356:ILE:HD13	2.43	0.48
1:B:209:ARG:HG3	1:B:210:TYR:O	2.13	0.48
1:B:197:ILE:HD11	1:B:222:VAL:HB	1.96	0.48
3:F:21:MET:HE3	3:F:74:ILE:HD11	1.94	0.48
3:F:83:ALA:HB3	3:F:85:TYR:HE1	1.78	0.48
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.48	0.48
2:E:124:THR:HA	2:E:154:PHE:O	2.13	0.48
1:B:215:ILE:N	1:B:215:ILE:HD13	2.28	0.48
1:B:284:HIS:O	1:B:287:ASN:HB3	2.13	0.48
3:F:32:ILE:CG2	3:F:89:GLN:HB3	2.44	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:85:TYR:HD1	3:F:85:TYR:N	2.11	0.48
2:E:35:SER:HB2	2:E:99:LEU:HD11	1.96	0.48
3:D:185:TYR:CE1	3:D:191:TYR:CE1	3.01	0.48
2:E:189:VAL:HG22	2:E:190:THR:N	2.29	0.48
1:A:403:ARG:NH2	1:B:29:ASP:O	2.46	0.48
1:A:65:MET:HE2	1:A:65:MET:HA	1.95	0.48
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.48	0.48
3:D:50:THR:HG23	3:D:70:TYR:CD2	2.49	0.48
1:B:379:PHE:CB	1:B:382:TYR:HD1	2.25	0.48
1:A:253:TRP:O	1:A:257:ILE:HD12	2.14	0.48
1:B:92:PHE:O	1:B:96:LEU:HB2	2.13	0.48
1:A:95:PHE:O	1:A:97:VAL:N	2.47	0.48
2:C:126:PRO:HA	2:C:210:SER:OG	2.13	0.48
3:D:32:ILE:HD13	3:D:50:THR:HA	1.95	0.48
1:A:127:VAL:O	1:A:128:LEU:C	2.52	0.48
3:F:72:LEU:HD23	3:F:73:THR:N	2.27	0.48
1:B:246:ASP:OD1	1:B:246:ASP:N	2.46	0.48
2:C:51:ILE:HD12	2:C:72:ARG:HG2	1.95	0.48
2:E:221:ARG:NH1	3:F:118:PRO:HD2	2.29	0.48
2:C:101:TYR:HA	2:C:107:TYR:CE2	2.49	0.48
3:F:48:TYR:O	3:F:52:LYS:HB2	2.14	0.48
1:A:150:PRO:HD3	1:A:354:GLY:CA	2.37	0.48
2:C:153:TYR:HD1	2:C:207:HIS:CD2	2.32	0.48
3:F:181:THR:HB	3:F:183:ASP:HB2	1.95	0.48
3:D:116:ILE:HD13	3:D:117:PHE:CA	2.44	0.48
3:F:123:GLN:O	3:F:123:GLN:HG2	2.13	0.48
2:E:104:GLY:O	2:E:106:TRP:HD1	1.96	0.48
1:B:264:ILE:HD12	1:B:265:PHE:N	2.29	0.48
3:F:12:SER:HA	3:F:104:GLU:O	2.14	0.48
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.43	0.47
3:F:33:HIS:CE1	3:F:49:ASP:N	2.81	0.47
3:D:162:TRP:N	3:D:162:TRP:HE3	2.12	0.47
1:A:75:TYR:O	1:A:78:LEU:HB2	2.14	0.47
1:A:98:ARG:HH22	1:A:102:PRO:HB3	1.78	0.47
1:B:126:ARG:O	1:B:130:VAL:HG23	2.14	0.47
3:D:119:PRO:HD3	3:D:131:VAL:HG22	1.96	0.47
1:B:434:LEU:HA	1:B:434:LEU:HD23	1.77	0.47
1:B:410:ILE:O	1:B:414:GLU:HG3	2.14	0.47
1:B:255:TYR:CG	1:B:424:PRO:HB3	2.49	0.47
1:A:451:ARG:O	1:A:455:LYS:HB2	2.14	0.47
2:C:30:SER:C	2:C:32:TYR:N	2.63	0.47
1:B:162:VAL:HG23	1:B:163:LEU:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:167:LEU:HD23	2:C:189:VAL:HG21	1.97	0.47
3:D:66:SER:HA	3:D:70:TYR:CE2	2.49	0.47
2:E:6:GLU:HA	2:E:22:CYS:HA	1.96	0.47
3:F:166:ASP:HB3	3:F:170:SER:H	1.78	0.47
2:E:33:TRP:CZ3	2:E:52:ASN:HB3	2.50	0.47
3:D:187:ARG:O	3:D:187:ARG:HG3	2.15	0.47
2:C:171:VAL:HG22	2:C:189:VAL:HG23	1.95	0.47
1:A:28:ARG:NE	1:B:207:GLN:HG2	2.29	0.47
1:A:57:VAL:CG1	1:A:139:LEU:HB3	2.44	0.47
1:B:409:ILE:HG21	1:B:426:ILE:HD11	1.96	0.47
1:B:257:ILE:HG22	1:B:371:PHE:HE1	1.75	0.47
2:E:28:ASP:O	2:E:30:SER:O	2.33	0.47
3:D:141:LYS:HB3	3:D:172:TYR:CE1	2.49	0.47
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.94	0.47
1:B:165:ILE:O	1:B:165:ILE:CG2	2.62	0.47
3:D:7:SER:OG	3:D:8:PRO:HD3	2.13	0.47
3:F:116:ILE:HA	3:F:132:VAL:O	2.15	0.47
1:A:391:ILE:O	1:A:391:ILE:HG22	2.15	0.47
1:B:260:ILE:HG23	1:B:435:LEU:CD1	2.45	0.47
2:C:129:VAL:CG1	2:C:205:VAL:HG21	2.45	0.47
1:A:276:MET:O	1:A:280:LEU:HB2	2.14	0.46
3:F:6:GLN:HE21	3:F:99:GLY:N	2.12	0.46
1:B:239:ILE:HD12	1:B:320:ILE:HB	1.97	0.46
1:B:348:PHE:CG	1:B:356:ILE:HD13	2.49	0.46
1:A:421:LEU:O	1:A:424:PRO:HD2	2.15	0.46
2:C:51:ILE:HD11	2:C:55:SER:CA	2.23	0.46
1:B:258:LEU:HD13	1:B:371:PHE:CD1	2.50	0.46
2:E:167:LEU:HD23	2:E:189:VAL:HG21	1.98	0.46
1:B:257:ILE:HG22	1:B:371:PHE:HZ	1.78	0.46
3:D:177:THR:HG22	3:D:178:LEU:N	2.31	0.46
2:E:107:TYR:C	2:E:107:TYR:CD1	2.89	0.46
2:E:107:TYR:C	2:E:107:TYR:HD1	2.19	0.46
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.16	0.46
1:A:337:PHE:O	1:A:341:VAL:HG23	2.15	0.46
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.51	0.46
3:F:146:LYS:HE3	3:F:153:GLU:CG	2.34	0.46
3:F:2:ILE:HG21	3:F:29:VAL:HG13	1.98	0.46
1:B:197:ILE:CD1	1:B:219:PHE:HD1	2.29	0.46
1:A:37:PHE:CD2	1:A:38:MET:HE1	2.50	0.46
1:A:271:LYS:HB2	1:A:271:LYS:HE3	1.77	0.46
1:B:287:ASN:HD21	1:B:290:LYS:H	1.53	0.46
1:A:427:ILE:CD1	1:A:427:ILE:H	2.27	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:122:VAL:HG21	1:B:160:ARG:HD3	1.98	0.46
2:C:131:PRO:HD3	2:C:216:LYS:HD2	1.98	0.46
1:B:397:LEU:HA	1:B:397:LEU:HD23	1.70	0.46
3:F:77:MET:CE	3:F:103:LEU:HD21	2.45	0.46
3:F:11:MET:HE1	3:F:19:VAL:HG13	1.98	0.46
1:A:427:ILE:HD13	1:A:427:ILE:H	1.81	0.46
2:E:67:LYS:HA	2:E:67:LYS:HD2	1.62	0.46
1:B:109:ILE:N	1:B:110:PRO:CD	2.79	0.46
2:E:57:THR:C	2:E:58:ILE:HD12	2.36	0.46
1:B:145:LEU:HD21	1:B:347:CYS:HB3	1.98	0.46
1:A:220:ILE:HG13	1:B:430:LEU:HD21	1.96	0.45
3:D:147:TRP:O	3:D:148:LYS:HG3	2.16	0.45
3:F:138:PHE:CD2	3:F:143:ILE:HD12	2.51	0.45
1:A:180:THR:HG22	1:A:218:VAL:CG2	2.46	0.45
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.97	0.45
3:D:47:ILE:HD12	3:D:47:ILE:N	2.32	0.45
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.73	0.45
2:E:180:ALA:O	2:E:181:ALA:HB3	2.17	0.45
1:A:46:VAL:HG13	1:A:155:GLY:HA2	1.98	0.45
1:A:270:ASN:HD21	1:A:401:SER:CB	2.29	0.45
3:D:89:GLN:O	3:D:95:GLN:HB2	2.16	0.45
1:A:37:PHE:CD2	1:A:38:MET:CE	2.90	0.45
1:B:42:VAL:HG22	1:B:162:VAL:HG21	1.99	0.45
1:B:262:PHE:CE2	1:B:396:ALA:HB3	2.52	0.45
3:D:192:THR:HA	3:D:207:SER:HB2	1.98	0.45
1:B:241:VAL:HG21	1:B:416:THR:CG2	2.44	0.45
1:A:109:ILE:CD1	1:A:149:GLY:HA2	2.46	0.45
1:A:356:ILE:O	1:A:360:MET:HE2	2.16	0.45
1:B:33:LEU:HD23	1:B:33:LEU:C	2.37	0.45
1:A:334:VAL:O	1:A:338:VAL:HG23	2.17	0.45
3:D:169:ASP:OD1	3:D:169:ASP:C	2.55	0.45
2:C:163:ASN:HD22	2:C:167:LEU:HD13	1.81	0.45
1:A:160:ARG:HD2	1:A:160:ARG:HA	1.75	0.45
1:A:437:GLN:HE21	1:B:216:LYS:HZ2	1.64	0.45
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.99	0.45
2:E:127:PRO:HA	2:E:153:TYR:HB3	1.98	0.45
1:A:407:THR:HG22	1:A:408:GLY:N	2.31	0.45
1:A:99:LYS:HG2	1:A:100:TYR:CZ	2.52	0.45
3:F:7:SER:OG	3:F:8:PRO:CD	2.46	0.45
2:C:98:ARG:HH11	2:C:110:VAL:HG21	1.81	0.45
1:A:107:SER:OG	1:A:109:ILE:CD1	2.61	0.45
3:D:32:ILE:N	3:D:32:ILE:CD1	2.78	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:311:ALA:HB3	1:B:336:ILE:CD1	2.47	0.45
3:F:148:LYS:HD2	3:F:194:GLU:OE2	2.16	0.45
2:E:38:ARG:HD3	2:E:94:TYR:CZ	2.52	0.45
1:A:131:LYS:CE	1:A:153:GLN:HE21	2.30	0.45
1:A:73:ASP:OD2	1:A:74:ASN:HB2	2.16	0.45
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.53	0.44
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.30	0.44
1:A:17:ARG:HE	1:A:17:ARG:C	2.20	0.44
1:B:345:LEU:O	1:B:346:LEU:C	2.55	0.44
3:F:32:ILE:HG22	3:F:89:GLN:CB	2.47	0.44
3:F:109:ASP:HB3	3:F:199:THR:HG21	1.98	0.44
1:A:305:LEU:C	1:A:307:PHE:N	2.70	0.44
3:D:10:ILE:HG23	3:D:102:LYS:HB3	2.00	0.44
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.99	0.44
3:F:116:ILE:HD13	3:F:193:CYS:HB2	2.00	0.44
1:A:430:LEU:CD1	1:B:219:PHE:CD2	2.79	0.44
2:C:127:PRO:HD2	2:C:212:THR:HG21	2.00	0.44
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.49	0.44
1:A:219:PHE:HZ	1:B:426:ILE:HD12	1.81	0.44
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.67	0.44
1:A:381:GLN:N	1:A:381:GLN:NE2	2.54	0.44
1:B:175:HIS:CB	1:B:213:ILE:CD1	2.92	0.44
1:B:213:ILE:HD13	1:B:213:ILE:N	2.32	0.44
2:E:69:ILE:HD12	2:E:69:ILE:N	2.31	0.44
1:B:88:VAL:HA	1:B:91:MET:HE2	2.00	0.44
1:B:336:ILE:O	1:B:340:ARG:HG3	2.17	0.44
3:D:107:ARG:CD	3:D:170:SER:HB2	2.48	0.44
1:A:244:LEU:HG	1:A:391:ILE:HD12	1.98	0.44
1:A:244:LEU:HB2	1:A:418:ASN:OD1	2.17	0.44
1:A:301:LEU:O	1:A:305:LEU:HG	2.17	0.44
3:D:65:GLY:O	3:D:66:SER:HB3	2.18	0.44
2:E:98:ARG:O	2:E:109:ASP:HB3	2.18	0.44
1:A:457:GLU:CG	1:B:18:ARG:HH11	2.30	0.44
1:B:198:LEU:HD12	1:B:406:LEU:HG	1.98	0.44
1:A:360:MET:HE1	1:A:402:ILE:HD11	2.00	0.44
1:B:317:PHE:HA	1:B:320:ILE:HD13	1.99	0.44
3:D:35:TYR:HE1	3:D:88:GLN:HB3	1.82	0.44
1:B:127:VAL:CB	1:B:157:ASN:ND2	2.74	0.44
2:E:104:GLY:O	2:E:106:TRP:CD1	2.71	0.44
2:C:39:GLN:O	2:C:92:ALA:HB1	2.17	0.44
3:F:84:THR:HA	3:F:102:LYS:HA	1.99	0.44
1:B:391:ILE:O	1:B:391:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:ILE:HD13	4:A:474:BR:BR	2.73	0.44
3:F:138:PHE:CE1	3:F:143:ILE:HD12	2.53	0.44
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.99	0.44
3:D:192:THR:HA	3:D:207:SER:HB3	1.98	0.44
2:E:108:PHE:HE1	3:F:88:GLN:HE21	1.65	0.44
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.83	0.44
3:D:77:MET:HG2	3:D:78:GLU:N	2.31	0.44
2:E:129:VAL:HB	2:E:214:VAL:HG11	1.98	0.44
3:D:115:SER:HB2	3:D:117:PHE:HE1	1.82	0.43
2:E:129:VAL:HG22	2:E:150:VAL:HG13	2.00	0.43
1:B:324:THR:HG23	1:B:390:ALA:HB3	2.00	0.43
2:E:185:LEU:C	2:E:185:LEU:HD12	2.38	0.43
3:F:6:GLN:HA	3:F:22:THR:O	2.18	0.43
3:F:184:GLU:CA	3:F:187:ARG:NH1	2.76	0.43
3:F:88:GLN:HB2	3:F:97:PHE:HD1	1.79	0.43
1:A:35:ILE:HD12	1:A:35:ILE:N	2.34	0.43
3:D:116:ILE:HD13	3:D:116:ILE:C	2.37	0.43
1:B:32:PRO:CG	1:B:35:ILE:HD13	2.48	0.43
1:B:138:THR:HG22	1:B:143:MET:SD	2.57	0.43
1:A:104:ALA:HB1	1:A:131:LYS:HD3	2.00	0.43
2:C:196:TRP:HA	2:C:198:SER:H	1.82	0.43
3:D:179:THR:HG22	3:D:180:LEU:N	2.34	0.43
2:E:57:THR:O	2:E:58:ILE:HG13	2.18	0.43
1:A:165:ILE:HG22	1:A:166:PHE:CE2	2.54	0.43
3:D:7:SER:CB	3:D:22:THR:HB	2.43	0.43
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.33	0.43
3:F:77:MET:HB2	3:F:77:MET:HE3	1.69	0.43
1:B:358:ALA:N	1:B:359:PRO:HD2	2.34	0.43
3:D:8:PRO:HG2	3:D:11:MET:SD	2.59	0.43
3:F:206:LYS:HD2	3:F:207:SER:H	1.83	0.43
2:E:36:TRP:CD1	2:E:70:ILE:HG13	2.52	0.43
3:F:8:PRO:O	3:F:10:ILE:N	2.51	0.43
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.53	0.43
2:C:163:ASN:CB	2:C:167:LEU:HD13	2.47	0.43
2:C:4:LEU:HD12	2:C:110:VAL:O	2.19	0.43
3:F:84:THR:OG1	3:F:102:LYS:HG2	2.19	0.43
3:F:95:GLN:O	3:F:96:THR:HG23	2.19	0.43
2:C:32:TYR:OH	2:C:98:ARG:NH2	2.43	0.43
3:D:9:ALA:C	3:D:10:ILE:HD13	2.38	0.43
1:B:264:ILE:C	1:B:264:ILE:HD12	2.39	0.43
3:F:88:GLN:HG2	3:F:89:GLN:N	2.34	0.43
3:D:136:ASN:CB	3:D:137:ASN:HD22	2.26	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:129:VAL:HG23	2:C:214:VAL:HG11	2.01	0.43
1:A:128:LEU:HA	1:A:154:ILE:CD1	2.48	0.43
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.83	0.42
2:C:93:LEU:HD11	2:C:114:GLY:HA3	2.01	0.42
1:A:447:ALA:O	1:A:451:ARG:HG2	2.18	0.42
1:B:305:LEU:C	1:B:307:PHE:N	2.72	0.42
1:B:445:LEU:HD12	1:B:445:LEU:HA	1.86	0.42
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.52	0.42
3:D:32:ILE:HD13	3:D:32:ILE:O	2.19	0.42
3:F:45:ARG:HG2	3:F:45:ARG:HH11	1.84	0.42
2:C:19:LYS:HD2	2:C:82:GLN:HE21	1.84	0.42
1:A:68:LEU:CD2	1:A:81:VAL:HG22	2.49	0.42
1:A:117:GLU:HG3	1:B:21:LEU:HD21	2.00	0.42
2:C:101:TYR:CA	2:C:107:TYR:CE2	3.02	0.42
1:A:332:MET:HE3	1:A:336:ILE:HD11	2.01	0.42
1:A:348:PHE:CD2	1:A:356:ILE:HD12	2.54	0.42
2:E:3:ARG:HH12	2:E:5:LEU:HG	1.85	0.42
1:B:194:LEU:HB2	1:B:414:GLU:OE2	2.20	0.42
1:A:360:MET:HE1	1:A:402:ILE:CD1	2.48	0.42
3:F:109:ASP:O	3:F:110:ALA:HB2	2.19	0.42
3:D:77:MET:CE	3:D:78:GLU:O	2.65	0.42
2:E:109:ASP:HA	3:F:45:ARG:HD3	1.99	0.42
3:D:60:ARG:NE	3:D:81:ASP:OD2	2.36	0.42
2:C:91:THR:HG22	2:C:91:THR:O	2.17	0.42
3:D:149:ILE:CG2	3:D:188:HIS:CG	3.02	0.42
1:A:109:ILE:N	1:A:110:PRO:HD2	2.35	0.42
1:A:73:ASP:CG	1:A:74:ASN:N	2.72	0.42
2:C:221:ARG:HG3	2:C:221:ARG:H	1.71	0.42
2:E:216:LYS:HB2	2:E:216:LYS:HE2	1.89	0.42
1:B:69:VAL:O	1:B:72:ALA:HB2	2.19	0.42
3:D:7:SER:HB2	3:D:22:THR:CA	2.49	0.42
1:B:305:LEU:C	1:B:307:PHE:H	2.21	0.42
3:F:138:PHE:HE2	3:F:174:MET:HB2	1.84	0.42
2:E:174:PHE:HZ	3:F:136:ASN:HD21	1.68	0.42
1:B:234:HIS:CD2	1:B:234:HIS:H	2.37	0.42
1:B:298:ILE:O	1:B:301:LEU:HB3	2.20	0.42
1:B:357:PHE:CE2	4:B:474:BR:BR	3.28	0.42
1:A:257:ILE:H	1:A:257:ILE:CD1	2.31	0.42
3:F:109:ASP:OD1	3:F:140:PRO:HD3	2.20	0.42
3:D:181:THR:OG1	3:D:184:GLU:CB	2.67	0.42
1:A:68:LEU:HD23	1:A:81:VAL:HG22	2.02	0.42
2:E:51:ILE:HG12	2:E:58:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:409:ILE:HG21	1:B:426:ILE:CD1	2.50	0.42
2:E:19:LYS:HA	2:E:81:LEU:O	2.19	0.42
1:A:457:GLU:CG	1:B:18:ARG:NH1	2.72	0.42
1:B:273:VAL:HA	1:B:345:LEU:HD22	2.01	0.42
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.85	0.42
1:B:64:ARG:NH1	1:B:141:GLY:O	2.53	0.42
3:F:116:ILE:HD11	3:F:147:TRP:CZ3	2.55	0.42
3:F:4:LEU:HD11	3:F:89:GLN:HG3	2.02	0.42
3:F:21:MET:HE1	3:F:74:ILE:HD11	2.01	0.42
1:B:199:PHE:HA	1:B:407:THR:OG1	2.20	0.42
1:A:206:PRO:HG2	1:A:211:THR:CG2	2.49	0.42
2:C:43:LYS:NZ	2:C:44:GLY:H	2.17	0.42
1:B:338:VAL:HG12	1:B:339:ALA:N	2.35	0.42
3:F:116:ILE:HD11	3:F:131:VAL:HG12	2.02	0.41
1:A:243:LYS:NZ	1:A:418:ASN:HA	2.35	0.41
3:F:180:LEU:HD22	3:F:184:GLU:HG2	2.01	0.41
3:F:189:ASN:HD21	3:F:210:ARG:H	1.67	0.41
1:B:86:SER:OG	1:B:303:GLY:HA3	2.20	0.41
1:A:230:ARG:O	1:A:234:HIS:HD2	2.03	0.41
3:D:30:SER:HA	3:D:70:TYR:OH	2.20	0.41
3:D:130:SER:HB3	3:D:177:THR:HG21	2.01	0.41
1:B:92:PHE:O	1:B:92:PHE:CD1	2.73	0.41
2:C:131:PRO:HD3	2:C:216:LYS:CD	2.50	0.41
2:C:29:TYR:CE2	2:C:72:ARG:NH1	2.87	0.41
2:E:20:LEU:HB2	2:E:81:LEU:HB3	2.02	0.41
3:F:149:ILE:HA	3:F:190:SER:O	2.20	0.41
3:D:187:ARG:O	3:D:188:HIS:CD2	2.73	0.41
1:B:391:ILE:O	1:B:391:ILE:CG2	2.68	0.41
3:F:32:ILE:HG22	3:F:89:GLN:CA	2.50	0.41
1:B:184:ALA:HB1	1:B:225:SER:CB	2.44	0.41
1:B:273:VAL:HG22	1:B:274:LEU:HD23	2.01	0.41
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.51	0.41
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.77	0.41
1:B:147:ARG:H	1:B:147:ARG:HG3	1.43	0.41
1:B:160:ARG:HH12	1:B:174:ARG:HD2	1.86	0.41
1:A:158:ILE:O	1:A:162:VAL:CG1	2.66	0.41
1:B:57:VAL:HG11	1:B:139:LEU:HB3	2.02	0.41
1:A:73:ASP:CG	1:A:74:ASN:H	2.21	0.41
2:E:204:ASN:HA	2:E:215:ASP:OD1	2.19	0.41
2:C:201:VAL:HG12	2:C:201:VAL:O	2.19	0.41
1:B:387:GLY:O	1:B:390:ALA:HB3	2.21	0.41
1:A:387:GLY:O	1:A:390:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:112:ILE:HD11	1:B:153:GLN:CG	2.50	0.41
1:B:255:TYR:CD1	1:B:424:PRO:HB3	2.55	0.41
1:A:356:ILE:HG22	4:A:474:BR:BR	2.75	0.41
3:F:107:ARG:NH1	3:F:171:THR:HG22	2.35	0.41
1:B:383:HIS:HB3	2:E:33:TRP:CZ2	2.56	0.41
1:B:423:LEU:HB3	1:B:424:PRO:HD3	2.03	0.41
1:B:183:ALA:HB2	1:B:200:ILE:CD1	2.50	0.41
2:C:156:GLU:OE2	2:C:176:ALA:CB	2.69	0.41
1:B:191:ASN:ND2	1:B:230:ARG:NH1	2.69	0.41
1:B:294:MET:O	1:B:298:ILE:HG12	2.20	0.41
1:B:287:ASN:ND2	1:B:289:THR:H	2.18	0.41
1:B:147:ARG:N	1:B:148:GLU:OE2	2.54	0.41
2:E:147:GLY:HA2	2:E:162:TRP:CH2	2.56	0.41
1:A:298:ILE:HG13	1:A:298:ILE:H	1.73	0.41
3:D:32:ILE:HD12	3:D:70:TYR:CD2	2.56	0.41
2:E:154:PHE:HA	2:E:155:PRO:HA	1.91	0.41
1:A:397:LEU:HA	1:A:397:LEU:HD23	1.79	0.41
1:A:241:VAL:HG12	1:A:244:LEU:CD2	2.51	0.41
3:D:149:ILE:HG12	3:D:191:TYR:HE2	1.85	0.41
3:F:187:ARG:HG2	3:F:188:HIS:CD2	2.56	0.41
1:B:257:ILE:CG2	1:B:371:PHE:HZ	2.34	0.41
1:B:98:ARG:HB3	1:B:288:ILE:CG1	2.49	0.41
1:B:336:ILE:HD13	1:B:336:ILE:HA	1.93	0.41
1:A:151:THR:OG1	1:A:189:ALA:HB2	2.21	0.41
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.66	0.41
1:A:219:PHE:CD2	1:B:430:LEU:HD13	2.51	0.41
1:A:32:PRO:CG	1:A:35:ILE:HD13	2.40	0.41
1:B:356:ILE:C	1:B:359:PRO:HD2	2.41	0.41
1:B:372:GLY:HA2	1:B:389:PHE:CD1	2.56	0.41
3:D:21:MET:H	3:D:21:MET:HG2	1.59	0.41
2:C:132:LEU:HB3	3:D:117:PHE:CD2	2.56	0.40
2:E:100:TYR:HB3	2:E:107:TYR:HE1	1.87	0.40
2:C:172:HIS:HE1	3:D:173:SER:OG	1.96	0.40
1:A:264:ILE:O	1:A:267:PRO:HD2	2.21	0.40
3:D:160:ASN:HB3	3:D:162:TRP:CZ3	2.55	0.40
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.36	0.40
1:A:420:GLN:HG3	1:A:420:GLN:H	1.41	0.40
3:F:187:ARG:CG	3:F:188:HIS:CD2	3.04	0.40
3:D:116:ILE:HD12	3:D:208:PHE:HD2	1.81	0.40
3:D:148:LYS:HB3	3:D:192:THR:HG23	2.03	0.40
1:A:435:LEU:HD22	1:A:435:LEU:HA	1.81	0.40
3:D:183:ASP:O	3:D:184:GLU:C	2.59	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:149:LEU:HD12	2:C:149:LEU:HA	1.92	0.40
1:A:29:ASP:OD1	1:B:403:ARG:NH2	2.42	0.40
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.71	0.40
2:C:111:TRP:N	2:C:111:TRP:CD1	2.89	0.40
1:B:110:PRO:HG3	1:B:448:ILE:CG2	2.52	0.40
3:D:116:ILE:CD1	3:D:117:PHE:N	2.66	0.40
1:A:143:MET:HB3	1:A:347:CYS:SG	2.62	0.40
1:A:266:GLY:O	1:A:270:ASN:ND2	2.55	0.40
2:E:153:TYR:CE1	2:E:183:TYR:HB3	2.57	0.40
1:A:100:TYR:O	1:A:101:ALA:HB2	2.21	0.40
3:D:80:GLU:H	3:D:80:GLU:HG3	1.50	0.40
3:F:197:HIS:O	3:F:198:LYS:C	2.60	0.40
1:B:162:VAL:CG2	1:B:163:LEU:N	2.84	0.40
2:C:48:ILE:HD11	2:C:94:TYR:CE1	2.56	0.40
3:F:115:SER:O	3:F:133:CYS:HA	2.20	0.40
3:D:137:ASN:ND2	3:D:137:ASN:N	2.70	0.40
1:B:28:ARG:HG2	1:B:29:ASP:N	2.36	0.40
1:B:38:MET:HA	1:B:41:VAL:HG13	2.04	0.40
1:B:435:LEU:HD22	1:B:435:LEU:HA	1.79	0.40
2:E:216:LYS:HA	2:E:216:LYS:HD3	1.83	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	442/473 (93%)	375 (85%)	59 (13%)	8 (2%)	13	61
1	B	439/473 (93%)	360 (82%)	68 (16%)	11 (2%)	9	51
2	C	219/221 (99%)	187 (85%)	18 (8%)	14 (6%)	2	20
2	E	219/221 (99%)	172 (78%)	37 (17%)	10 (5%)	4	31
3	D	209/211 (99%)	167 (80%)	30 (14%)	12 (6%)	3	24
3	F	209/211 (99%)	169 (81%)	25 (12%)	15 (7%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1737/1810 (96%)	1430 (82%)	237 (14%)	70 (4%)	5	36

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
2	C	43	LYS
2	C	135	GLY
2	C	139	ALA
2	C	168	ALA
3	D	7	SER
3	D	50	THR
3	D	169	ASP
3	D	198	LYS
2	E	3	ARG
2	E	62	PRO
2	E	65	LYS
2	E	122	ALA
2	E	138	ALA
2	E	195	SER
3	F	7	SER
3	F	8	PRO
3	F	49	ASP
3	F	50	THR
3	F	108	ALA
3	F	183	ASP
3	F	198	LYS
1	A	96	LEU
1	B	96	LEU
1	B	288	ILE
1	B	387	GLY
2	C	42	GLY
2	C	65	LYS
3	D	62	SER
3	D	126	SER
3	D	187	ARG
2	E	179	GLN
3	F	54	THR
3	F	98	GLY
1	A	74	ASN
1	B	317	PHE
1	B	444	LEU

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Mol	Chain	Res	Type
2	C	44	GLY
2	C	138	ALA
2	C	140	ALA
3	D	66	SER
3	F	102	LYS
3	F	151	GLY
1	A	411	LEU
2	C	31	ARG
3	D	64	SER
3	D	120	SER
2	E	135	GLY
3	F	112	PRO
1	A	332	MET
1	B	73	ASP
1	B	165	ILE
1	B	332	MET
2	C	85	LYS
2	C	197	PRO
2	E	41	PRO
3	F	76	THR
1	B	206	PRO
1	B	398	LEU
2	E	137	ALA
3	F	9	ALA
1	A	288	ILE
2	C	52	ASN
2	C	62	PRO
1	A	101	ALA
1	A	231	ILE
1	B	231	ILE
3	D	203	PRO
3	D	151	GLY
3	F	119	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/358 (94%)	283 (84%)	52 (16%)	4	19
1	B	332/358 (93%)	275 (83%)	57 (17%)	3	15
2	C	181/181 (100%)	143 (79%)	38 (21%)	1	8
2	E	181/181 (100%)	143 (79%)	38 (21%)	1	8
3	D	185/185 (100%)	147 (80%)	38 (20%)	2	8
3	F	185/185 (100%)	150 (81%)	35 (19%)	2	11
All	All	1399/1448 (97%)	1141 (82%)	258 (18%)	2	12

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	19	ARG
1	A	30	LYS
1	A	31	THR
1	A	44	THR
1	A	60	LEU
1	A	62	ASN
1	A	65	MET
1	A	74	ASN
1	A	81	VAL
1	A	96	LEU
1	A	103	GLU
1	A	122	VAL
1	A	126	ARG
1	A	171	ASP
1	A	201	ILE
1	A	205	ARG
1	A	207	GLN
1	A	209	ARG
1	A	211	THR
1	A	212	LEU
1	A	219	PHE
1	A	225	SER
1	A	226	THR
1	A	244	LEU
1	A	261	ILE
1	A	264	ILE
1	A	270	ASN
1	A	278	ASP
1	A	279	LEU

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Mol	Chain	Res	Type
1	A	289	THR
1	A	293	LEU
1	A	319	LEU
1	A	336	ILE
1	A	338	VAL
1	A	346	LEU
1	A	377	GLU
1	A	378	LEU
1	A	381	GLN
1	A	398	LEU
1	A	407	THR
1	A	420	GLN
1	A	423	LEU
1	A	427	ILE
1	A	433	THR
1	A	435	LEU
1	A	437	GLN
1	A	444	LEU
1	A	445	LEU
1	A	451	ARG
1	A	452	THR
1	A	453	LEU
1	B	19	ARG
1	B	41	VAL
1	B	44	THR
1	B	62	ASN
1	B	65	MET
1	B	69	VAL
1	B	77	LEU
1	B	81	VAL
1	B	84	LEU
1	B	85	CYS
1	B	86	SER
1	B	92	PHE
1	B	95	PHE
1	B	96	LEU
1	B	103	GLU
1	B	122	VAL
1	B	138	THR
1	B	139	LEU
1	B	147	ARG
1	B	148	GLU

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Mol	Chain	Res	Type
1	B	169	LYS
1	B	180	THR
1	B	202	GLU
1	B	205	ARG
1	B	207	GLN
1	B	208	PHE
1	B	211	THR
1	B	212	LEU
1	B	215	ILE
1	B	219	PHE
1	B	236	VAL
1	B	241	VAL
1	B	246	ASP
1	B	251	THR
1	B	273	VAL
1	B	279	LEU
1	B	284	HIS
1	B	304	LEU
1	B	313	SER
1	B	327	ASN
1	B	334	VAL
1	B	338	VAL
1	B	376	VAL
1	B	377	GLU
1	B	378	LEU
1	B	381	GLN
1	B	397	LEU
1	B	398	LEU
1	B	401	SER
1	B	402	ILE
1	B	420	GLN
1	B	435	LEU
1	B	444	LEU
1	B	445	LEU
1	B	451	ARG
1	B	453	LEU
1	B	457	GLU
2	C	2	VAL
2	C	3	ARG
2	C	5	LEU
2	C	12	VAL
2	C	21	SER

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Mol	Chain	Res	Type
2	C	22	CYS
2	C	30	SER
2	C	31	ARG
2	C	43	LYS
2	C	51	ILE
2	C	65	LYS
2	C	72	ARG
2	C	84	SER
2	C	89	GLU
2	C	98	ARG
2	C	100	TYR
2	C	110	VAL
2	C	115	THR
2	C	121	SER
2	C	129	VAL
2	C	142	SER
2	C	145	THR
2	C	150	VAL
2	C	151	LYS
2	C	178	LEU
2	C	185	LEU
2	C	186	SER
2	C	187	SER
2	C	193	SER
2	C	195	SER
2	C	199	GLU
2	C	200	THR
2	C	204	ASN
2	C	213	LYS
2	C	214	VAL
2	C	217	LYS
2	C	219	VAL
2	C	221	ARG
3	D	1	ASP
3	D	5	THR
3	D	32	ILE
3	D	39	SER
3	D	41	THR
3	D	42	SER
3	D	44	LYS
3	D	46	TRP
3	D	50	THR

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Mol	Chain	Res	Type
3	D	59	VAL
3	D	68	THR
3	D	71	SER
3	D	76	THR
3	D	80	GLU
3	D	115	SER
3	D	116	ILE
3	D	125	THR
3	D	135	LEU
3	D	136	ASN
3	D	137	ASN
3	D	143	ILE
3	D	145	VAL
3	D	146	LYS
3	D	152	SER
3	D	156	ASN
3	D	159	LEU
3	D	162	TRP
3	D	169	ASP
3	D	175	SER
3	D	181	THR
3	D	186	GLU
3	D	189	ASN
3	D	192	THR
3	D	196	THR
3	D	200	SER
3	D	201	THR
3	D	202	SER
3	D	206	LYS
2	E	2	VAL
2	E	3	ARG
2	E	4	LEU
2	E	5	LEU
2	E	7	SER
2	E	12	VAL
2	E	21	SER
2	E	31	ARG
2	E	34	MET
2	E	51	ILE
2	E	54	VAL
2	E	57	THR
2	E	59	ASN

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Mol	Chain	Res	Type
2	E	66	ASP
2	E	69	ILE
2	E	70	ILE
2	E	78	THR
2	E	84	SER
2	E	96	CYS
2	E	98	ARG
2	E	107	TYR
2	E	115	THR
2	E	116	THR
2	E	117	VAL
2	E	123	LYS
2	E	128	SER
2	E	136	SER
2	E	151	LYS
2	E	173	THR
2	E	177	VAL
2	E	178	LEU
2	E	182	LEU
2	E	190	THR
2	E	193	SER
2	E	199	GLU
2	E	200	THR
2	E	211	SER
2	E	219	VAL
3	F	5	THR
3	F	27	SER
3	F	36	GLN
3	F	41	THR
3	F	55	SER
3	F	59	VAL
3	F	60	ARG
3	F	68	THR
3	F	85	TYR
3	F	86	TYR
3	F	88	GLN
3	F	97	PHE
3	F	103	LEU
3	F	107	ARG
3	F	120	SER
3	F	125	THR
3	F	133	CYS

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Mol	Chain	Res	Type
3	F	143	ILE
3	F	144	ASN
3	F	146	LYS
3	F	152	SER
3	F	155	GLN
3	F	164	ASP
3	F	168	LYS
3	F	174	MET
3	F	175	SER
3	F	177	THR
3	F	179	THR
3	F	180	LEU
3	F	181	THR
3	F	187	ARG
3	F	189	ASN
3	F	192	THR
3	F	196	THR
3	F	206	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	74	ASN
1	A	119	GLN
1	A	153	GLN
1	A	157	ASN
1	A	233	ASN
1	A	270	ASN
1	A	277	GLN
1	A	284	HIS
1	A	287	ASN
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	A	460	GLN
1	B	62	ASN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	234	HIS
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	277	GLN
1	B	284	HIS
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	420	GLN
2	C	163	ASN
2	C	172	HIS
3	D	6	GLN
3	D	37	GLN
3	D	136	ASN
3	D	137	ASN
3	D	144	ASN
3	D	165	GLN
3	D	188	HIS
3	D	189	ASN
3	F	6	GLN
3	F	33	HIS
3	F	88	GLN
3	F	136	ASN
3	F	137	ASN
3	F	189	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	444/473 (93%)	-0.31	0 100 100	39, 82, 124, 180	0
1	B	441/473 (93%)	-0.32	0 100 100	31, 80, 122, 192	0
2	C	221/221 (100%)	-0.30	0 100 100	36, 74, 135, 184	0
2	E	221/221 (100%)	-0.21	0 100 100	39, 87, 144, 178	0
3	D	211/211 (100%)	-0.18	0 100 100	40, 91, 132, 155	0
3	F	211/211 (100%)	-0.16	0 100 100	29, 80, 144, 179	0
All	All	1749/1810 (96%)	-0.27	0 100 100	29, 82, 136, 192	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BR	A	475	1/1	0.47	12.16	78,78,78,78	0
4	BR	A	474	1/1	0.55	10.39	78,78,78,78	0
4	BR	B	475	1/1	0.45	9.15	78,78,78,78	0
4	BR	B	474	1/1	0.52	8.55	78,78,78,78	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.