



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 01:46 PM EDT

PDB ID : 2EZ0  
Title : Crystal structure of the S107A/E148Q/Y445A mutant of EcClC, in complex with a FaB fragment  
Authors : Lobet, S.; Dutzler, R.  
Deposited on : 2005-11-10  
Resolution : 3.54 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

<https://www.wwpdb.org/validation/2017/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:

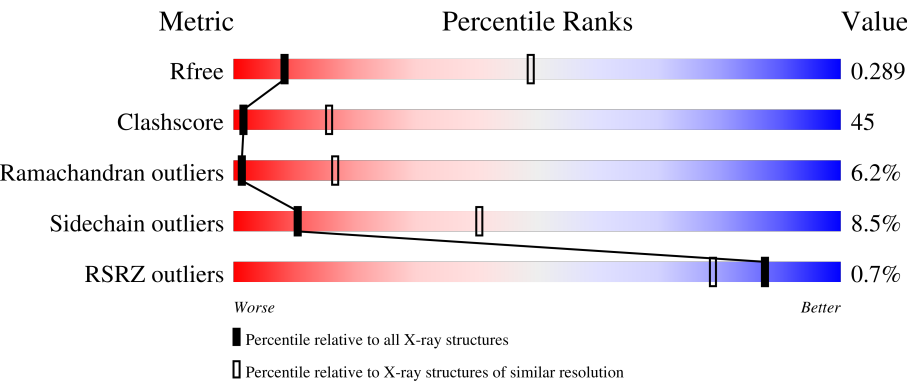
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.54 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 <sub>free</sub>	130704	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	473	<div><div>2%</div><div>34%52%7%6%</div></div>
1	B	473	<div><div>33%52%8%7%</div></div>
2	C	222	<div><div>2%</div><div>41%48%10%</div></div>
2	E	222	<div><div>45%44%10%</div></div>
3	D	211	<div><div>44%48%8%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	211	 38% 52% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	A	474	-	-	X	-
4	BR	B	474	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13209 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3325	2184	561	560	20			
1	B	441	Total	C	N	O	S	0	0	0
			3296	2168	554	554	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	SER	engineered mutation	UNP P37019
A	148	GLN	GLU	engineered mutation	UNP P37019
A	445	ALA	TYR	engineered mutation	UNP P37019
B	107	ALA	SER	engineered mutation	UNP P37019
B	148	GLN	GLU	engineered mutation	UNP P37019
B	445	ALA	TYR	engineered mutation	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			

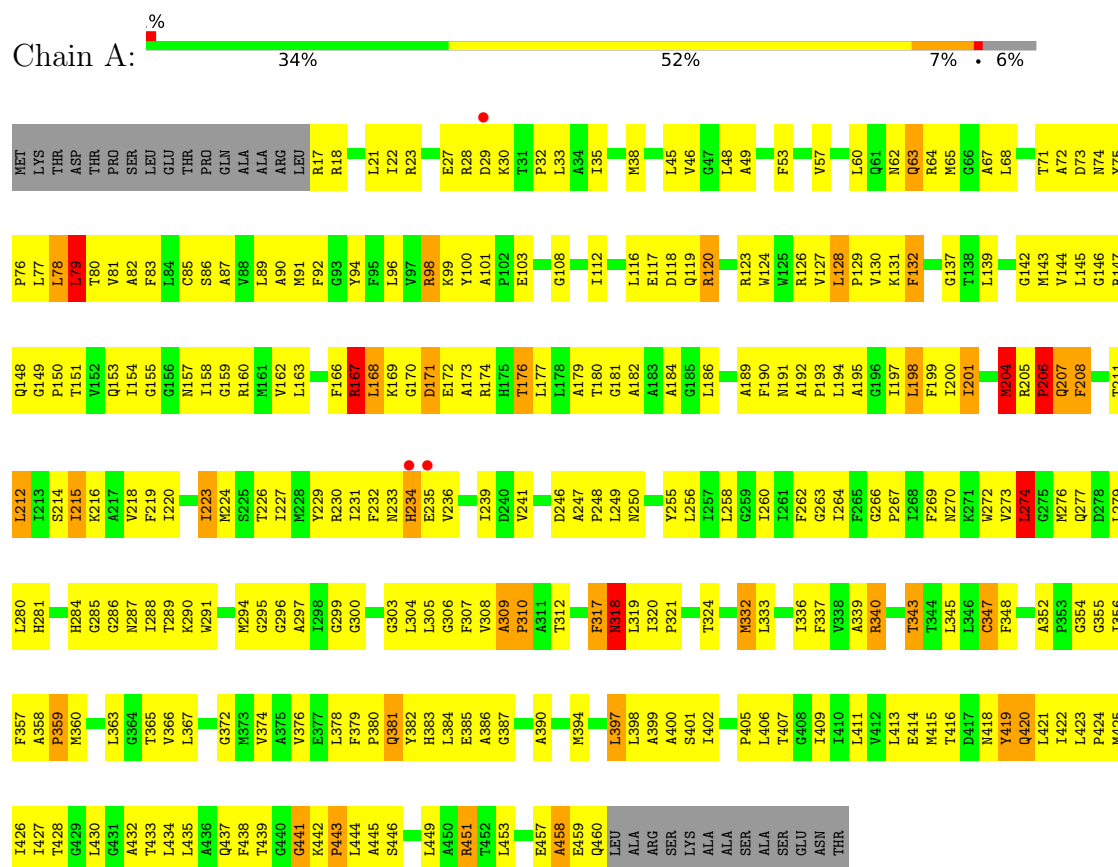
- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Br 1	0	0
4	B	1	Total 1	Br 1	0	0

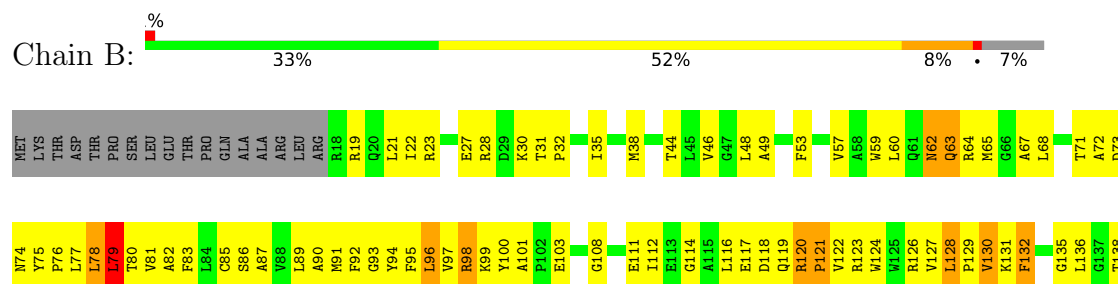
### 3 Residue-property plots

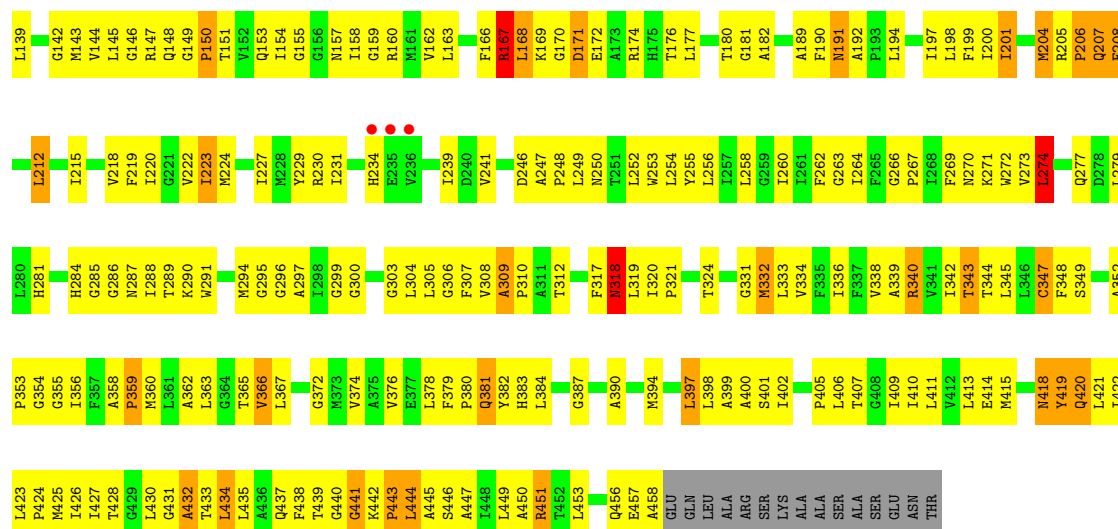
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

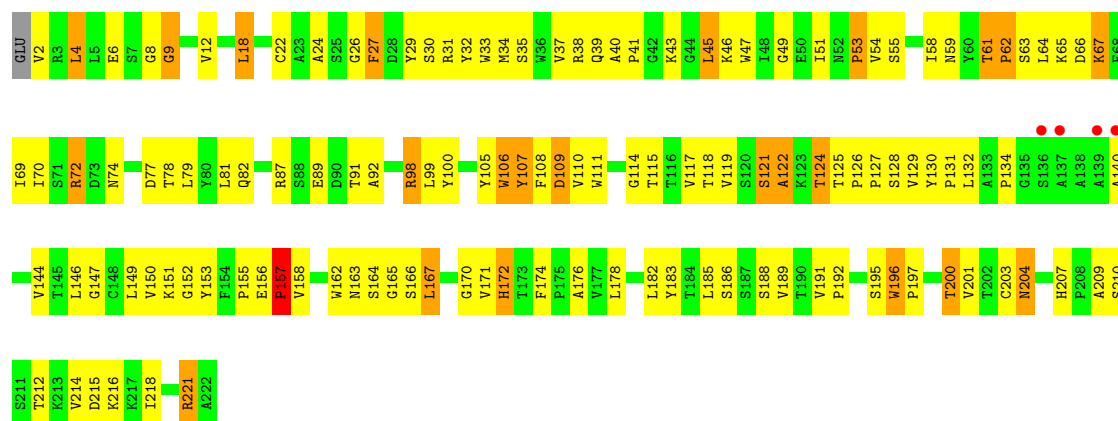
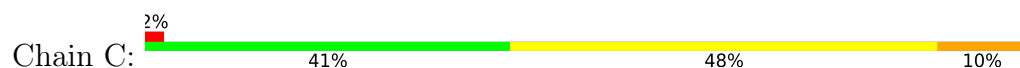


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

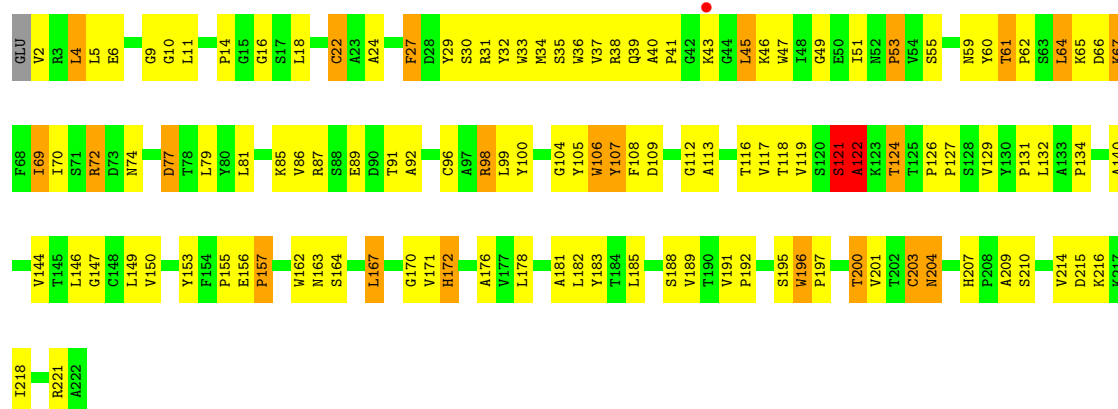




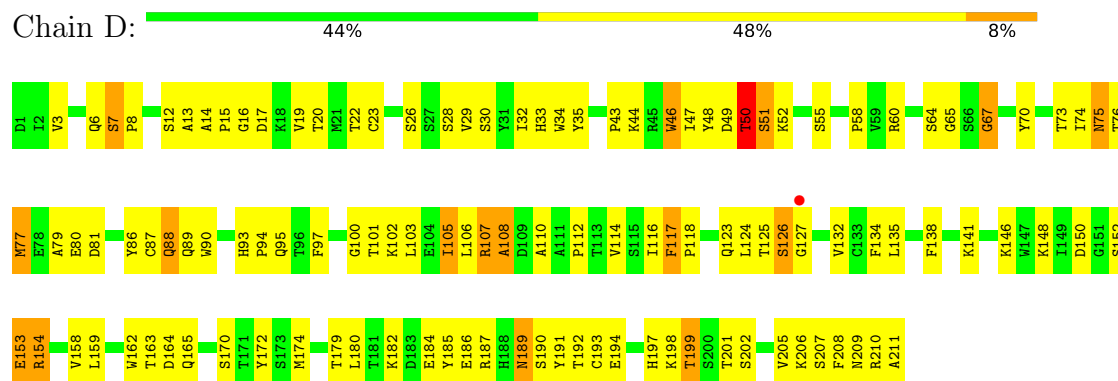
● Molecule 2: Fab Fragment (Heavy Chain)



● Molecule 2: Fab Fragment (Heavy Chain)



## ● Molecule 3: Fab Fragment (Light Chain)



## ● Molecule 3: Fab Fragment (Light Chain)





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.16Å 124.03Å 149.28Å 90.00° 127.97° 90.00°	Depositor
Resolution (Å)	19.92 – 3.54 20.42 – 3.54	Depositor EDS
% Data completeness (in resolution range)	87.1 (19.92-3.54) 87.1 (20.42-3.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.53Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.258 , 0.296 0.252 , 0.289	Depositor DCC
$R_{free}$ test set	1680 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.2	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 87.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	13209	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.57	0/3396	0.74	1/4609 (0.0%)
1	B	0.57	0/3367	0.74	0/4571
2	C	0.86	5/1721 (0.3%)	0.83	2/2355 (0.1%)
2	E	0.86	3/1721 (0.2%)	0.90	5/2355 (0.2%)
3	D	0.75	3/1660 (0.2%)	0.82	3/2257 (0.1%)
3	F	0.81	2/1660 (0.1%)	0.80	1/2257 (0.0%)
All	All	0.71	13/13525 (0.1%)	0.79	12/18404 (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
3	D	0	1
3	F	0	2
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	107	ARG	C-N	12.37	1.62	1.34
3	D	107	ARG	C-O	-11.78	1.00	1.23
3	D	108	ALA	CA-CB	8.25	1.69	1.52
2	E	122	ALA	CA-CB	8.01	1.69	1.52
2	C	121	SER	CA-CB	7.67	1.64	1.52
2	C	121	SER	C-N	-6.84	1.18	1.34
2	C	61	THR	CB-CG2	-6.59	1.30	1.52
2	E	121	SER	CA-C	-6.51	1.36	1.52
3	F	102	LYS	CE-NZ	-6.07	1.33	1.49
2	E	121	SER	C-N	5.42	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	102	LYS	CE-NZ	-5.19	1.36	1.49
2	C	121	SER	CA-C	-5.13	1.39	1.52
2	C	63	SER	C-N	-5.04	1.22	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	107	ARG	CA-C-O	10.98	143.16	120.10
2	E	121	SER	CA-C-N	-10.94	93.13	117.20
3	D	50	THR	O-C-N	-9.37	107.70	122.70
3	D	107	ARG	CA-C-N	-8.82	97.79	117.20
3	F	50	THR	O-C-N	-8.21	109.56	122.70
2	E	121	SER	C-N-CA	-7.29	103.47	121.70
2	E	121	SER	N-CA-C	7.21	130.47	111.00
2	E	121	SER	CA-C-O	7.06	134.93	120.10
2	C	121	SER	O-C-N	5.92	132.17	122.70
1	A	204	MET	CA-CB-CG	-5.43	104.06	113.30
2	C	121	SER	CA-C-N	-5.43	105.25	117.20
2	E	122	ALA	CB-CA-C	-5.34	102.09	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	50	THR	Mainchain
3	F	31	TYR	Sidechain
3	F	50	THR	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3325	0	3482	354	0
1	B	3296	0	3455	370	0
2	C	1672	0	1654	143	0
2	E	1672	0	1654	125	0
3	D	1621	0	1546	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1621	0	1546	140	0
4	A	1	0	0	3	0
4	B	1	0	0	3	0
All	All	13209	0	13337	1191	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 45.

All (1191) 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)
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.28	1.12
1:A:18:ARG:NH2	1:B:456:GLN:HE21	1.54	1.05
1:A:68:LEU:HD21	1:A:82:ALA:HB2	1.39	1.04
1:B:68:LEU:HD21	1:B:82:ALA:HB2	1.41	1.03
1:B:413:LEU:HD12	1:B:422:ILE:HD13	1.40	1.03
3:F:192:THR:HA	3:F:207:SER:HB3	1.41	1.02
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.41	1.01
1:B:120:ARG:HB3	1:B:120:ARG:HH11	1.20	1.01
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.42	1.01
1:A:381:GLN:H	1:A:381:GLN:HE21	1.01	0.98
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.44	0.97
3:D:192:THR:HA	3:D:207:SER:HB3	1.45	0.96
1:B:143:MET:HB3	1:B:347:CYS:SG	2.06	0.95
2:C:45:LEU:HD12	2:C:45:LEU:H	1.33	0.93
2:E:45:LEU:HD12	2:E:45:LEU:H	1.34	0.93
1:B:381:GLN:H	1:B:381:GLN:HE21	0.94	0.93
1:A:120:ARG:HH11	1:A:120:ARG:HB3	1.35	0.92
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.50	0.92
1:A:143:MET:HB3	1:A:347:CYS:SG	2.10	0.91
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.50	0.91
1:B:250:ASN:HD22	2:E:105:TYR:HE1	1.17	0.91
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.53	0.90
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.55	0.89
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.33	0.89
1:B:381:GLN:HE21	1:B:381:GLN:N	1.71	0.88
1:A:413:LEU:HD12	1:A:422:ILE:HD13	1.52	0.88
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.55	0.88
1:A:119:GLN:HB3	1:A:453:LEU:HD11	1.55	0.88
2:C:172:HIS:HB2	2:C:188:SER:HB3	1.55	0.88
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.56	0.88
3:F:110:ALA:O	3:F:138:PHE:HA	1.74	0.88
1:B:381:GLN:H	1:B:381:GLN:NE2	1.72	0.87
1:B:120:ARG:HH11	1:B:120:ARG:CB	1.87	0.87
3:F:2:ILE:HD11	3:F:27:SER:HB2	1.57	0.87
1:A:374:VAL:HG12	1:A:378:LEU:HD12	1.55	0.86
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.37	0.86
1:A:332:MET:O	1:A:336:ILE:HG13	1.76	0.85
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.58	0.85
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.57	0.85
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.57	0.85
1:B:374:VAL:HG12	1:B:378:LEU:HD12	1.56	0.85
1:B:145:LEU:HD13	1:B:354:GLY:HA3	1.58	0.85
2:C:132:LEU:HD21	3:D:132:VAL:HG21	1.58	0.85
1:B:48:LEU:H	1:B:48:LEU:HD22	1.42	0.84
3:F:14:ALA:O	3:F:17:ASP:HB2	1.77	0.84
1:A:274:LEU:O	1:A:277:GLN:HG2	1.78	0.84
1:B:274:LEU:O	1:B:277:GLN:HG2	1.78	0.83
1:A:145:LEU:HD13	1:A:354:GLY:HA3	1.60	0.83
1:A:199:PHE:HE2	1:A:204:MET:HE2	1.44	0.83
1:B:120:ARG:HB3	1:B:120:ARG:NH1	1.93	0.82
1:A:421:LEU:O	1:A:425:MET:HG3	1.80	0.81
2:C:207:HIS:HE1	2:C:209:ALA:HB3	1.45	0.81
3:D:95:GLN:OE1	3:D:95:GLN:N	2.13	0.81
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.63	0.80
2:E:91:THR:OG1	2:E:119:VAL:HG23	1.81	0.80
1:B:38:MET:HG3	1:B:168:LEU:HD21	1.64	0.80
1:A:381:GLN:H	1:A:381:GLN:NE2	1.77	0.80
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.16	0.80
1:B:98:ARG:NH1	1:B:98:ARG:HB3	1.97	0.79
3:F:82:ALA:HB2	3:F:105:ILE:HD11	1.65	0.79
1:B:320:ILE:HG21	1:B:394:MET:CE	2.13	0.79
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.17	0.79
1:A:150:PRO:O	1:A:154:ILE:HG13	1.83	0.79
1:A:320:ILE:HG23	1:A:365:THR:HG21	1.64	0.79
1:A:38:MET:HG3	1:A:168:LEU:HD21	1.65	0.79
1:A:405:PRO:O	1:A:409:ILE:HG12	1.83	0.79
3:D:189:ASN:HD21	3:D:211:ALA:H	1.29	0.78
1:B:119:GLN:HB3	1:B:453:LEU:HD11	1.64	0.78
1:A:381:GLN:HE21	1:A:381:GLN:N	1.78	0.78
2:E:207:HIS:CE1	2:E:209:ALA:HB3	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:HA2	1:A:153:GLN:NE2	1.98	0.77
1:A:144:VAL:HG21	1:A:343:THR:HB	1.67	0.77
1:A:320:ILE:HG21	1:A:394:MET:CE	2.14	0.77
2:E:41:PRO:HD3	2:E:92:ALA:HA	1.67	0.77
3:F:189:ASN:HD21	3:F:211:ALA:H	1.32	0.77
2:E:121:SER:O	2:E:122:ALA:O	2.03	0.77
2:C:2:VAL:HA	2:C:26:GLY:HA3	1.66	0.76
1:A:120:ARG:HH11	1:A:120:ARG:CB	1.97	0.76
1:A:199:PHE:HE2	1:A:204:MET:CE	1.99	0.76
1:A:250:ASN:HD22	2:C:105:TYR:HE1	1.33	0.76
2:E:207:HIS:HE1	2:E:209:ALA:HB3	1.50	0.76
1:A:28:ARG:HG3	1:B:208:PHE:HZ	1.51	0.76
1:A:98:ARG:HB3	1:A:98:ARG:NH1	2.01	0.76
3:F:192:THR:CA	3:F:207:SER:HB3	2.16	0.76
3:D:14:ALA:O	3:D:17:ASP:HB2	1.84	0.75
1:B:144:VAL:HG21	1:B:343:THR:HB	1.68	0.75
2:C:132:LEU:HB2	2:C:147:GLY:O	1.86	0.75
1:B:182:ALA:HB1	1:B:204:MET:HE1	1.68	0.75
1:A:457:GLU:HG3	1:A:458:ALA:N	2.01	0.75
2:E:172:HIS:HB2	2:E:188:SER:HB3	1.69	0.74
3:F:150:ASP:HA	3:F:190:SER:HB3	1.69	0.74
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.70	0.73
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.06	0.73
1:A:159:GLY:O	1:A:162:VAL:HG22	1.88	0.72
1:B:320:ILE:HG23	1:B:365:THR:HG21	1.70	0.72
3:D:150:ASP:HA	3:D:190:SER:HB3	1.69	0.72
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.71	0.72
2:E:24:ALA:HB1	2:E:27:PHE:HE1	1.55	0.72
3:F:77:MET:SD	3:F:103:LEU:HD21	2.29	0.72
2:C:72:ARG:NH1	2:C:74:ASN:OD1	2.23	0.72
1:B:320:ILE:HD13	1:B:394:MET:HE2	1.70	0.71
2:C:51:ILE:HD11	2:C:55:SER:HB3	1.71	0.71
2:C:189:VAL:HG13	2:C:189:VAL:O	1.90	0.71
1:B:98:ARG:HB3	1:B:98:ARG:HH11	1.54	0.71
3:D:30:SER:HA	3:D:70:TYR:OH	1.90	0.71
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.55	0.71
1:B:90:ALA:HB3	1:B:296:GLY:HA2	1.73	0.71
2:C:124:THR:HG22	2:C:125:THR:N	2.06	0.71
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.91	0.71
3:F:111:ALA:HB2	3:F:199:THR:HB	1.73	0.71
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PRO:HD2	1:A:381:GLN:NE2	2.05	0.71
1:A:163:LEU:HD21	1:A:174:ARG:HG3	1.73	0.70
3:D:192:THR:CA	3:D:207:SER:HB3	2.20	0.70
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.27	0.70
3:F:95:GLN:N	3:F:95:GLN:OE1	2.23	0.70
3:F:111:ALA:N	3:F:199:THR:HG21	2.06	0.70
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.26	0.70
1:A:18:ARG:NH2	1:B:456:GLN:NE2	2.34	0.70
1:B:199:PHE:HE2	1:B:204:MET:HE2	1.56	0.70
1:B:87:ALA:O	1:B:91:MET:HG3	1.91	0.70
1:A:451:ARG:HH11	1:A:451:ARG:HB3	1.57	0.69
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.27	0.69
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.57	0.69
1:B:159:GLY:O	1:B:162:VAL:HG22	1.91	0.69
2:C:126:PRO:HB3	2:C:210:SER:OG	1.91	0.69
1:B:46:VAL:O	1:B:49:ALA:HB3	1.91	0.69
1:B:108:GLY:HA2	1:B:153:GLN:NE2	2.08	0.69
2:C:41:PRO:HD3	2:C:92:ALA:HA	1.75	0.69
2:C:129:VAL:HG21	2:C:214:VAL:CG2	2.23	0.69
2:C:185:LEU:O	2:C:185:LEU:HD12	1.92	0.69
2:E:11:LEU:HB3	2:E:124:THR:HG23	1.75	0.69
3:F:148:LYS:HB2	3:F:192:THR:OG1	1.93	0.69
1:A:163:LEU:HD12	1:A:168:LEU:CD1	2.23	0.69
1:A:444:LEU:O	1:A:444:LEU:HD13	1.92	0.69
1:B:380:PRO:HD2	1:B:381:GLN:NE2	2.07	0.69
1:A:231:ILE:HD13	1:B:249:LEU:CD1	2.24	0.69
1:A:199:PHE:CE2	1:A:204:MET:CE	2.76	0.68
1:B:420:GLN:NE2	1:B:421:LEU:HG	2.08	0.68
1:B:287:ASN:HD22	1:B:290:LYS:N	1.90	0.68
1:B:332:MET:O	1:B:336:ILE:HG13	1.94	0.68
1:A:269:PHE:O	1:A:273:VAL:HG12	1.92	0.68
3:F:30:SER:HA	3:F:70:TYR:OH	1.93	0.68
1:A:208:PHE:HZ	1:B:28:ARG:HG3	1.59	0.68
1:A:318:ASN:HD22	1:A:319:LEU:N	1.91	0.68
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.74	0.68
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.58	0.68
1:B:444:LEU:HD13	1:B:444:LEU:O	1.93	0.68
1:A:420:GLN:NE2	1:A:421:LEU:HG	2.09	0.68
3:D:7:SER:HB3	3:D:8:PRO:CD	2.23	0.68
1:B:172:GLU:HG3	1:B:212:LEU:HB3	1.76	0.68
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:148:LYS:HA	3:F:152:SER:O	1.94	0.68
1:B:227:ILE:O	1:B:231:ILE:HG12	1.94	0.68
1:B:287:ASN:HD22	1:B:290:LYS:H	1.37	0.68
2:E:39:GLN:O	2:E:92:ALA:HB1	1.94	0.68
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.75	0.68
1:A:120:ARG:HB3	1:A:120:ARG:NH1	2.07	0.67
1:A:422:ILE:HA	1:A:425:MET:HE3	1.75	0.67
3:D:182:LYS:HG2	3:D:186:GLU:OE1	1.94	0.67
2:E:126:PRO:HB3	2:E:210:SER:OG	1.95	0.67
3:F:7:SER:HB3	3:F:8:PRO:CD	2.22	0.67
1:A:98:ARG:HB3	1:A:98:ARG:HH11	1.59	0.67
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.77	0.67
2:E:72:ARG:NH1	2:E:74:ASN:OD1	2.28	0.67
2:E:204:ASN:HB3	2:E:215:ASP:OD1	1.95	0.67
3:F:192:THR:HA	3:F:207:SER:CB	2.23	0.67
1:B:312:THR:HG22	1:B:339:ALA:CB	2.24	0.67
1:A:48:LEU:H	1:A:48:LEU:HD22	1.60	0.67
1:B:355:GLY:HA3	4:B:474:BR:BR	2.51	0.66
1:A:266:GLY:HA3	1:A:400:ALA:HB1	1.77	0.66
1:A:255:TYR:HB3	1:A:428:THR:OG1	1.96	0.66
1:A:287:ASN:HD22	1:A:290:LYS:H	1.43	0.66
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.30	0.66
2:C:192:PRO:O	2:C:195:SER:HB3	1.95	0.66
2:E:129:VAL:HG21	2:E:214:VAL:CG2	2.26	0.66
1:A:180:THR:HG22	1:A:218:VAL:HA	1.77	0.66
1:A:124:TRP:HA	1:A:157:ASN:ND2	2.10	0.66
1:B:163:LEU:HD12	1:B:168:LEU:CD1	2.25	0.66
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.61	0.66
3:F:194:GLU:CG	3:F:205:VAL:HG12	2.24	0.66
1:B:267:PRO:O	1:B:270:ASN:HB2	1.95	0.66
2:C:132:LEU:HD21	3:D:132:VAL:CG2	2.26	0.66
1:A:87:ALA:O	1:A:91:MET:HG3	1.96	0.65
3:D:148:LYS:HA	3:D:152:SER:O	1.96	0.65
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.79	0.65
3:F:179:THR:O	3:F:180:LEU:HD23	1.97	0.65
1:B:163:LEU:HD21	1:B:174:ARG:HG3	1.77	0.65
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.62	0.65
1:B:212:LEU:HD12	1:B:212:LEU:N	2.11	0.65
1:B:279:LEU:O	1:B:279:LEU:HD23	1.97	0.65
2:E:18:LEU:HD23	2:E:18:LEU:H	1.61	0.65
2:C:124:THR:HG22	2:C:125:THR:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HH11	1:A:451:ARG:CB	2.10	0.65
1:B:266:GLY:HA3	1:B:400:ALA:HB1	1.79	0.64
1:B:451:ARG:HB3	1:B:451:ARG:HH11	1.61	0.64
2:E:6:GLU:HA	2:E:22:CYS:HA	1.78	0.64
1:A:96:LEU:O	1:A:130:VAL:HG13	1.97	0.64
3:F:111:ALA:HB2	3:F:199:THR:CB	2.27	0.64
1:A:320:ILE:HD13	1:A:394:MET:HE2	1.78	0.64
1:B:250:ASN:ND2	2:E:105:TYR:CE1	2.65	0.64
3:D:22:THR:HG22	3:D:23:CYS:N	2.12	0.64
1:A:65:MET:C	1:A:67:ALA:H	1.98	0.64
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.26	0.64
3:D:13:ALA:HB3	3:D:77:MET:CE	2.27	0.64
1:B:19:ARG:HG2	1:B:19:ARG:HH11	1.63	0.64
1:B:65:MET:C	1:B:67:ALA:H	2.01	0.64
2:C:18:LEU:HD23	2:C:18:LEU:H	1.63	0.64
1:B:451:ARG:HH11	1:B:451:ARG:CB	2.11	0.63
3:F:15:PRO:HD3	3:F:105:ILE:HG22	1.79	0.63
3:D:107:ARG:NE	3:D:108:ALA:O	2.30	0.63
3:F:22:THR:HG22	3:F:23:CYS:N	2.14	0.63
3:F:32:ILE:HG22	3:F:33:HIS:N	2.14	0.63
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.17	0.63
1:A:172:GLU:HG3	1:A:212:LEU:HB3	1.79	0.63
1:B:124:TRP:HA	1:B:157:ASN:ND2	2.11	0.63
2:C:45:LEU:HD12	2:C:45:LEU:N	2.09	0.63
3:F:7:SER:CB	3:F:8:PRO:HD3	2.24	0.63
1:B:190:PHE:O	1:B:192:ALA:N	2.31	0.63
1:A:46:VAL:O	1:A:49:ALA:HB3	1.98	0.63
1:A:148:GLN:HB3	1:A:190:PHE:CE1	2.33	0.63
1:B:374:VAL:HG12	1:B:378:LEU:CD1	2.27	0.63
2:C:12:VAL:CG2	2:C:119:VAL:HG22	2.28	0.63
1:B:212:LEU:HD12	1:B:212:LEU:H	1.62	0.63
1:A:227:ILE:O	1:A:231:ILE:HG12	1.99	0.62
1:B:150:PRO:O	1:B:154:ILE:HG13	1.99	0.62
2:E:134:PRO:O	2:E:221:ARG:HG3	1.99	0.62
2:E:185:LEU:HD12	2:E:185:LEU:O	1.98	0.62
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.16	0.62
2:E:45:LEU:HD12	2:E:45:LEU:N	2.11	0.62
1:A:27:GLU:OE2	1:A:30:LYS:HD2	1.99	0.62
2:C:149:LEU:HD12	2:C:150:VAL:N	2.15	0.62
1:B:68:LEU:O	1:B:78:LEU:HD21	2.00	0.62
1:A:182:ALA:HB1	1:A:204:MET:HE1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:HG12	1:A:378:LEU:CD1	2.28	0.62
2:C:196:TRP:HB3	2:C:197:PRO:HD3	1.81	0.62
3:F:197:HIS:ND1	3:F:198:LYS:N	2.48	0.62
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.35	0.62
1:A:267:PRO:O	1:A:270:ASN:HB2	1.98	0.61
1:A:226:THR:HG21	1:B:423:LEU:HD13	1.82	0.61
2:C:35:SER:HB2	2:C:49:GLY:O	2.00	0.61
2:E:49:GLY:HA3	2:E:70:ILE:CD1	2.29	0.61
1:A:260:ILE:O	1:A:264:ILE:HG23	2.00	0.61
1:B:191:ASN:HB2	1:B:229:TYR:CE2	2.35	0.61
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.27	0.61
2:E:192:PRO:O	2:E:195:SER:HB3	1.99	0.61
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.81	0.61
3:D:7:SER:CB	3:D:8:PRO:HD3	2.27	0.61
2:E:132:LEU:HB2	2:E:147:GLY:O	2.01	0.61
3:F:134:PHE:O	3:F:135:LEU:HD23	2.01	0.61
2:C:185:LEU:HD12	2:C:185:LEU:C	2.21	0.61
1:B:148:GLN:HB3	1:B:190:PHE:CE1	2.36	0.61
2:C:6:GLU:HA	2:C:22:CYS:HA	1.81	0.61
1:B:53:PHE:O	1:B:57:VAL:HG23	2.01	0.61
2:E:127:PRO:HB3	2:E:153:TYR:CB	2.31	0.61
2:E:129:VAL:HG21	2:E:214:VAL:HG21	1.83	0.61
1:B:21:LEU:C	1:B:21:LEU:HD23	2.21	0.60
1:B:86:SER:OG	1:B:303:GLY:HA3	2.00	0.60
1:B:120:ARG:HD3	1:B:453:LEU:CD1	2.31	0.60
2:E:106:TRP:HD1	2:E:106:TRP:H	1.48	0.60
1:A:21:LEU:HD23	1:A:21:LEU:C	2.21	0.60
1:A:458:ALA:N	1:A:460:GLN:HE22	1.99	0.60
1:B:423:LEU:HB3	1:B:424:PRO:HD3	1.82	0.60
1:A:108:GLY:HA2	1:A:153:GLN:HE21	1.65	0.60
1:A:287:ASN:HD21	1:A:289:THR:HB	1.66	0.60
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.15	0.60
1:B:405:PRO:O	1:B:409:ILE:HG12	2.01	0.60
2:E:129:VAL:CG2	2:E:214:VAL:HG21	2.32	0.60
1:A:124:TRP:CA	1:A:157:ASN:HD22	2.09	0.60
2:C:30:SER:C	2:C:32:TYR:H	2.04	0.60
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.83	0.60
1:B:72:ALA:HA	1:B:78:LEU:HD11	1.84	0.60
2:E:51:ILE:CD1	2:E:72:ARG:HD2	2.31	0.60
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.31	0.60
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PHE:O	1:B:191:ASN:C	2.37	0.60
2:E:30:SER:C	2:E:32:TYR:H	2.03	0.60
1:B:421:LEU:C	1:B:425:MET:HE2	2.22	0.60
1:B:441:GLY:O	1:B:442:LYS:HG3	2.01	0.60
2:E:2:VAL:HG23	2:E:2:VAL:O	2.02	0.60
1:A:356:ILE:HG12	1:A:356:ILE:O	2.02	0.60
1:A:441:GLY:C	1:A:442:LYS:HG3	2.22	0.60
1:B:287:ASN:HD21	1:B:289:THR:HB	1.67	0.59
3:F:114:VAL:HG13	3:F:135:LEU:HD23	1.84	0.59
1:B:333:LEU:HD22	1:B:366:VAL:HG13	1.84	0.59
2:C:45:LEU:HD11	3:D:86:TYR:CD1	2.37	0.59
2:E:91:THR:HG23	2:E:118:THR:HA	1.83	0.59
2:E:189:VAL:HG13	2:E:189:VAL:O	2.02	0.59
1:B:382:TYR:HB3	1:B:384:LEU:HD21	1.84	0.59
1:B:399:ALA:O	1:B:433:THR:HG23	2.02	0.59
1:B:101:ALA:HB2	1:B:130:VAL:HG21	1.83	0.59
1:A:287:ASN:HD22	1:A:290:LYS:N	1.99	0.59
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.33	0.59
1:B:269:PHE:O	1:B:273:VAL:HG12	2.03	0.59
3:D:205:VAL:O	3:D:206:LYS:HG2	2.03	0.59
1:A:199:PHE:HA	1:A:407:THR:OG1	2.01	0.59
3:F:158:VAL:O	3:F:159:LEU:HD23	2.03	0.58
2:C:91:THR:HG23	2:C:118:THR:HA	1.84	0.58
3:F:29:VAL:CG2	3:F:32:ILE:HD11	2.33	0.58
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.85	0.58
1:B:318:ASN:HD22	1:B:319:LEU:N	2.01	0.58
2:C:129:VAL:CG2	2:C:214:VAL:HG21	2.33	0.58
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.86	0.58
3:D:29:VAL:CG2	3:D:32:ILE:HD11	2.34	0.58
3:D:179:THR:O	3:D:180:LEU:HD23	2.02	0.58
1:A:92:PHE:O	1:A:96:LEU:HD23	2.03	0.58
3:D:192:THR:HA	3:D:207:SER:CB	2.26	0.58
1:B:92:PHE:O	1:B:96:LEU:HD23	2.03	0.58
1:B:199:PHE:HA	1:B:407:THR:OG1	2.03	0.58
2:C:18:LEU:HD23	2:C:18:LEU:N	2.18	0.58
3:D:114:VAL:HG22	3:D:135:LEU:CD2	2.32	0.58
1:B:423:LEU:HG	1:B:427:ILE:HD11	1.86	0.58
1:A:28:ARG:HG3	1:B:208:PHE:CZ	2.35	0.58
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.39	0.58
3:D:197:HIS:ND1	3:D:198:LYS:N	2.51	0.58
2:E:10:GLY:N	2:E:116:THR:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:182:LYS:HG2	3:F:186:GLU:OE1	2.03	0.58
1:B:38:MET:HG3	1:B:168:LEU:CD2	2.33	0.58
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.86	0.58
1:A:75:TYR:HB3	1:A:76:PRO:CD	2.30	0.57
1:A:148:GLN:NE2	1:A:189:ALA:HB1	2.19	0.57
1:A:320:ILE:HG23	1:A:365:THR:CG2	2.34	0.57
3:D:20:THR:HG23	3:D:73:THR:OG1	2.04	0.57
1:A:171:ASP:HA	1:A:174:ARG:NH1	2.19	0.57
1:A:208:PHE:CZ	1:B:28:ARG:HG3	2.40	0.57
2:C:127:PRO:HB3	2:C:153:TYR:CB	2.32	0.57
3:D:117:PHE:CD1	3:D:117:PHE:N	2.72	0.57
1:A:401:SER:O	1:A:444:LEU:HB3	2.04	0.57
1:B:199:PHE:CE2	1:B:204:MET:CE	2.88	0.57
1:A:305:LEU:C	1:A:307:PHE:H	2.07	0.57
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.85	0.57
1:B:284:HIS:O	1:B:286:GLY:N	2.37	0.57
1:B:420:GLN:HE22	1:B:421:LEU:HG	1.69	0.57
2:C:129:VAL:HG21	2:C:214:VAL:HG21	1.86	0.57
1:A:17:ARG:HD2	1:A:17:ARG:C	2.24	0.57
1:A:357:PHE:HB3	4:A:474:BR:BR	2.59	0.57
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.39	0.57
2:E:51:ILE:HD11	2:E:55:SER:HB3	1.84	0.57
3:F:114:VAL:HG12	3:F:115:SER:N	2.19	0.57
1:A:86:SER:OG	1:A:303:GLY:HA3	2.03	0.57
1:B:96:LEU:O	1:B:130:VAL:HG13	2.05	0.57
1:B:260:ILE:O	1:B:264:ILE:HG23	2.04	0.57
2:E:40:ALA:HA	2:E:92:ALA:CB	2.34	0.57
1:B:167:ARG:O	1:B:168:LEU:C	2.42	0.57
3:D:210:ARG:HG2	3:D:210:ARG:HH11	1.68	0.57
2:E:146:LEU:HD13	2:E:218:ILE:HG21	1.86	0.57
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.87	0.56
1:A:382:TYR:HB3	1:A:384:LEU:HD21	1.87	0.56
1:A:420:GLN:HE22	1:A:421:LEU:HG	1.69	0.56
2:C:200:THR:HG22	2:C:200:THR:O	2.05	0.56
1:A:355:GLY:HA3	4:A:474:BR:BR	2.59	0.56
2:E:18:LEU:HD23	2:E:18:LEU:N	2.18	0.56
1:A:18:ARG:O	1:A:18:ARG:HG2	2.06	0.56
1:A:79:LEU:H	1:A:79:LEU:HD23	1.70	0.56
1:A:348:PHE:CD1	1:A:356:ILE:HB	2.41	0.56
1:B:421:LEU:C	1:B:424:PRO:HD2	2.25	0.56
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.87	0.56
2:E:35:SER:HB2	2:E:49:GLY:O	2.05	0.56
2:E:51:ILE:HD13	2:E:72:ARG:HD2	1.87	0.56
2:E:196:TRP:HB3	2:E:197:PRO:HD3	1.87	0.56
3:F:20:THR:HG23	3:F:73:THR:OG1	2.06	0.56
3:F:88:GLN:HB2	3:F:97:PHE:HD1	1.69	0.56
1:A:98:ARG:HB2	1:A:288:ILE:HG13	1.88	0.56
1:A:119:GLN:CB	1:A:453:LEU:HD11	2.32	0.56
1:A:320:ILE:HG21	1:A:394:MET:HE1	1.87	0.56
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.21	0.56
1:B:79:LEU:HD23	1:B:79:LEU:H	1.70	0.56
1:B:441:GLY:C	1:B:442:LYS:HG3	2.26	0.56
3:D:127:GLY:O	3:D:182:LYS:N	2.33	0.56
1:A:72:ALA:HA	1:A:78:LEU:HD11	1.86	0.56
1:B:320:ILE:HG21	1:B:394:MET:HE1	1.87	0.56
1:B:163:LEU:HD12	1:B:168:LEU:HD12	1.88	0.56
1:B:255:TYR:HB3	1:B:428:THR:OG1	2.05	0.56
2:C:204:ASN:HB3	2:C:215:ASP:OD1	2.05	0.56
3:F:58:PRO:C	3:F:60:ARG:H	2.08	0.56
1:A:241:VAL:HG12	1:A:241:VAL:O	2.04	0.56
1:B:108:GLY:HA2	1:B:153:GLN:HE21	1.71	0.56
1:B:205:ARG:O	1:B:207:GLN:N	2.39	0.56
2:C:100:TYR:HB3	2:C:107:TYR:CE1	2.41	0.56
3:D:95:GLN:CD	3:D:95:GLN:H	2.08	0.56
1:A:249:LEU:CD1	1:B:231:ILE:HD13	2.36	0.56
2:E:207:HIS:ND1	2:E:210:SER:HB3	2.21	0.56
1:A:239:ILE:HG22	1:A:241:VAL:HG23	1.87	0.56
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.87	0.56
1:A:457:GLU:C	1:A:459:GLU:H	2.09	0.56
2:E:178:LEU:HB2	2:E:183:TYR:CE2	2.41	0.56
3:F:107:ARG:NH2	3:F:108:ALA:O	2.39	0.56
1:A:53:PHE:O	1:A:57:VAL:HG23	2.06	0.55
1:A:94:TYR:OH	1:A:352:ALA:HB2	2.06	0.55
1:A:284:HIS:HA	1:A:290:LYS:HB3	1.88	0.55
1:A:68:LEU:O	1:A:78:LEU:HD21	2.06	0.55
1:B:27:GLU:OE2	1:B:30:LYS:HD2	2.06	0.55
1:B:199:PHE:CE2	1:B:204:MET:HE2	2.37	0.55
3:F:116:ILE:HD13	3:F:193:CYS:CB	2.36	0.55
2:C:51:ILE:HD13	2:C:72:ARG:HD2	1.88	0.55
1:A:163:LEU:HD12	1:A:168:LEU:HD12	1.88	0.55
1:A:212:LEU:N	1:A:212:LEU:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:61:THR:HB	2:E:62:PRO:CD	2.36	0.55
1:A:74:ASN:O	1:A:77:LEU:HB3	2.05	0.55
1:A:90:ALA:HB3	1:A:296:GLY:HA2	1.89	0.55
1:A:199:PHE:CE2	1:A:204:MET:HE2	2.32	0.55
1:A:422:ILE:O	1:A:426:ILE:HG13	2.06	0.55
1:A:166:PHE:O	1:A:168:LEU:N	2.40	0.55
1:B:119:GLN:CB	1:B:453:LEU:HD11	2.37	0.55
2:C:163:ASN:ND2	2:C:167:LEU:HD23	2.22	0.55
3:F:95:GLN:H	3:F:95:GLN:CD	2.10	0.55
3:F:153:GLU:HG3	3:F:154:ARG:H	1.72	0.55
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.41	0.55
1:A:284:HIS:C	1:A:286:GLY:H	2.10	0.55
2:C:51:ILE:CD1	2:C:72:ARG:HD2	2.37	0.55
3:F:115:SER:HB3	3:F:117:PHE:CE1	2.42	0.55
3:F:116:ILE:CD1	3:F:193:CYS:HB2	2.37	0.55
3:F:210:ARG:HH11	3:F:210:ARG:HG2	1.71	0.55
2:E:49:GLY:HA3	2:E:70:ILE:HD12	1.89	0.55
3:F:190:SER:HA	3:F:209:ASN:OD1	2.06	0.55
1:A:176:THR:HG22	1:A:177:LEU:N	2.22	0.54
1:A:78:LEU:O	1:A:79:LEU:C	2.46	0.54
2:C:2:VAL:O	2:C:2:VAL:HG13	2.08	0.54
1:A:419:TYR:CE1	1:A:422:ILE:HG21	2.43	0.54
3:F:13:ALA:HB3	3:F:77:MET:CE	2.37	0.54
1:A:372:GLY:O	1:A:376:VAL:HG23	2.07	0.54
3:F:79:ALA:HA	3:F:105:ILE:HD13	1.89	0.54
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.42	0.54
1:A:205:ARG:O	1:A:207:GLN:N	2.40	0.54
1:A:398:LEU:HD22	1:A:402:ILE:HG21	1.88	0.54
1:B:418:ASN:O	1:B:420:GLN:N	2.40	0.54
2:C:196:TRP:O	2:C:197:PRO:C	2.43	0.54
1:A:98:ARG:HD3	1:A:291:TRP:CE3	2.42	0.54
1:A:223:ILE:HG22	1:A:224:MET:N	2.23	0.54
1:B:320:ILE:HG23	1:B:365:THR:CG2	2.35	0.54
2:C:109:ASP:OD2	2:C:110:VAL:HG23	2.07	0.54
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.33	0.54
3:D:158:VAL:O	3:D:159:LEU:HD23	2.07	0.54
1:A:65:MET:C	1:A:67:ALA:N	2.61	0.54
1:B:145:LEU:HD13	1:B:354:GLY:CA	2.36	0.54
1:A:18:ARG:HH21	1:B:456:GLN:HE21	1.49	0.54
1:B:358:ALA:HB3	1:B:359:PRO:CD	2.38	0.54
1:A:86:SER:HB2	1:A:300:GLY:HA2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD12	1:A:212:LEU:H	1.72	0.53
1:B:305:LEU:C	1:B:307:PHE:H	2.10	0.53
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.89	0.53
3:F:72:LEU:C	3:F:72:LEU:HD23	2.27	0.53
1:A:190:PHE:O	1:A:191:ASN:C	2.46	0.53
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.90	0.53
1:A:284:HIS:O	1:A:286:GLY:N	2.41	0.53
1:B:267:PRO:HB3	1:B:441:GLY:HA3	1.90	0.53
3:D:190:SER:HA	3:D:209:ASN:OD1	2.09	0.53
1:A:383:HIS:CD2	2:C:33:TRP:CE3	2.93	0.53
1:A:423:LEU:HG	1:A:427:ILE:HD11	1.90	0.53
1:B:21:LEU:HD23	1:B:22:ILE:N	2.23	0.53
1:B:64:ARG:NH1	1:B:64:ARG:HB3	2.24	0.53
1:B:176:THR:HG22	1:B:177:LEU:N	2.22	0.53
1:B:340:ARG:HA	1:B:343:THR:OG1	2.07	0.53
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.08	0.53
3:D:46:TRP:HA	3:D:46:TRP:CE3	2.43	0.53
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.43	0.53
1:A:312:THR:HG22	1:A:339:ALA:CB	2.39	0.53
1:B:284:HIS:C	1:B:286:GLY:H	2.12	0.53
3:D:153:GLU:HG3	3:D:154:ARG:H	1.73	0.53
1:A:167:ARG:O	1:A:168:LEU:C	2.47	0.53
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.43	0.53
1:A:144:VAL:HG21	1:A:343:THR:CB	2.38	0.53
1:A:171:ASP:HA	1:A:174:ARG:HH12	1.73	0.53
1:A:216:LYS:HD3	1:B:434:LEU:CD2	2.39	0.53
1:B:180:THR:HG22	1:B:218:VAL:HA	1.91	0.53
2:E:70:ILE:HG12	2:E:81:LEU:HD13	1.91	0.53
1:A:449:LEU:O	1:A:453:LEU:N	2.42	0.53
1:B:331:GLY:O	1:B:333:LEU:N	2.42	0.53
3:F:205:VAL:O	3:F:206:LYS:HG2	2.09	0.53
1:A:383:HIS:HE1	3:D:90:TRP:CZ2	2.26	0.53
1:B:98:ARG:HD3	1:B:291:TRP:CE3	2.44	0.53
1:B:199:PHE:HE2	1:B:204:MET:CE	2.19	0.53
1:B:241:VAL:HG12	1:B:241:VAL:O	2.09	0.53
2:C:30:SER:O	2:C:32:TYR:N	2.42	0.53
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.91	0.53
3:F:6:GLN:HG3	3:F:100:GLY:H	1.74	0.53
1:A:35:ILE:O	1:A:38:MET:N	2.39	0.53
1:A:367:LEU:HD12	1:A:367:LEU:O	2.08	0.53
1:B:270:ASN:O	1:B:273:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD12	1:B:438:PHE:CE2	2.44	0.53
3:D:134:PHE:O	3:D:135:LEU:HD23	2.09	0.53
1:A:120:ARG:HD3	1:A:453:LEU:CD1	2.39	0.52
1:A:308:VAL:O	1:A:309:ALA:HB2	2.08	0.52
1:A:318:ASN:C	1:A:318:ASN:ND2	2.62	0.52
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.91	0.52
2:E:40:ALA:HA	2:E:92:ALA:HB2	1.91	0.52
2:E:107:TYR:HB3	3:F:33:HIS:NE2	2.24	0.52
1:A:60:LEU:O	1:A:64:ARG:HG3	2.09	0.52
1:B:148:GLN:HG3	1:B:190:PHE:CZ	2.44	0.52
2:C:40:ALA:HA	2:C:92:ALA:CB	2.38	0.52
2:E:39:GLN:C	2:E:92:ALA:HB1	2.28	0.52
1:A:78:LEU:HA	1:A:81:VAL:HG22	1.91	0.52
1:B:85:CYS:O	1:B:89:LEU:HG	2.09	0.52
1:A:270:ASN:O	1:A:273:VAL:HG13	2.09	0.52
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.91	0.52
1:A:145:LEU:HD13	1:A:354:GLY:CA	2.36	0.52
1:A:158:ILE:O	1:A:162:VAL:HG13	2.09	0.52
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.45	0.52
1:A:419:TYR:CG	1:A:419:TYR:O	2.61	0.52
2:C:49:GLY:HA3	2:C:70:ILE:CD1	2.40	0.52
2:E:207:HIS:CE1	2:E:210:SER:H	2.28	0.52
3:F:29:VAL:HG21	3:F:32:ILE:HD11	1.92	0.52
1:A:85:CYS:O	1:A:89:LEU:HG	2.10	0.52
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.90	0.52
1:A:360:MET:SD	1:A:397:LEU:CD1	2.98	0.52
1:B:284:HIS:HA	1:B:290:LYS:HB3	1.92	0.52
1:B:312:THR:HG22	1:B:339:ALA:HB1	1.91	0.52
2:C:99:LEU:HD21	2:C:108:PHE:CD2	2.44	0.52
3:F:111:ALA:CA	3:F:199:THR:HG21	2.40	0.52
2:C:39:GLN:O	2:C:92:ALA:HB1	2.10	0.52
1:A:180:THR:O	1:A:181:GLY:C	2.49	0.52
1:A:216:LYS:HD3	1:B:434:LEU:HD22	1.91	0.52
1:A:309:ALA:H	1:A:310:PRO:HD3	1.75	0.52
1:B:117:GLU:O	1:B:118:ASP:HB2	2.10	0.52
1:B:146:GLY:HA3	1:B:358:ALA:HB3	1.92	0.52
1:B:207:GLN:HB3	1:B:208:PHE:CE1	2.44	0.52
1:B:318:ASN:HD22	1:B:318:ASN:C	2.13	0.52
2:C:24:ALA:HB1	2:C:27:PHE:HE1	1.74	0.52
3:F:29:VAL:HG23	3:F:70:TYR:CE1	2.45	0.52
1:B:171:ASP:HA	1:B:174:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:THR:HG23	1:B:390:ALA:HB3	1.91	0.52
2:E:67:LYS:HE2	2:E:85:LYS:O	2.10	0.52
1:A:18:ARG:HH21	1:B:456:GLN:NE2	2.06	0.52
1:A:18:ARG:HH12	1:B:457:GLU:HB3	1.75	0.52
1:A:356:ILE:O	1:A:360:MET:HG3	2.10	0.52
1:A:418:ASN:O	1:A:420:GLN:N	2.43	0.52
2:C:91:THR:HA	2:C:117:VAL:O	2.10	0.51
3:D:58:PRO:C	3:D:60:ARG:H	2.13	0.51
2:E:144:VAL:O	2:E:144:VAL:HG13	2.10	0.51
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.92	0.51
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.92	0.51
2:E:149:LEU:HD12	2:E:150:VAL:N	2.26	0.51
3:F:47:ILE:HG22	3:F:48:TYR:N	2.26	0.51
1:B:65:MET:C	1:B:67:ALA:N	2.62	0.51
1:B:362:ALA:O	1:B:366:VAL:HG23	2.11	0.51
3:F:19:VAL:HG12	3:F:74:ILE:HB	1.91	0.51
1:A:139:LEU:HD13	1:A:147:ARG:HB3	1.93	0.51
1:B:86:SER:HB2	1:B:300:GLY:HA2	1.92	0.51
2:C:40:ALA:HA	2:C:92:ALA:HB2	1.92	0.51
2:E:132:LEU:HB3	3:F:117:PHE:CD2	2.45	0.51
1:A:383:HIS:CE1	3:D:90:TRP:CZ2	2.99	0.51
1:B:98:ARG:CZ	1:B:291:TRP:CZ3	2.94	0.51
2:C:22:CYS:O	2:C:78:THR:HG23	2.10	0.51
2:C:124:THR:CG2	2:C:125:THR:N	2.73	0.51
3:D:50:THR:O	3:D:51:SER:HB3	2.11	0.51
1:A:23:ARG:HG3	1:A:23:ARG:NH1	2.26	0.51
1:B:98:ARG:HB2	1:B:288:ILE:HG13	1.92	0.51
1:B:270:ASN:O	1:B:273:VAL:CG1	2.58	0.51
1:A:198:LEU:HD21	1:B:198:LEU:HD11	1.92	0.51
1:A:457:GLU:C	1:A:459:GLU:N	2.63	0.51
1:B:79:LEU:H	1:B:79:LEU:CD2	2.24	0.51
3:D:112:PRO:HB3	3:D:138:PHE:HB3	1.92	0.51
1:A:198:LEU:CD2	1:B:406:LEU:HD21	2.40	0.51
1:A:318:ASN:HD22	1:A:318:ASN:C	2.08	0.51
1:A:333:LEU:HD22	1:A:366:VAL:HG13	1.92	0.51
1:B:101:ALA:CB	1:B:130:VAL:HG21	2.41	0.51
1:B:372:GLY:O	1:B:376:VAL:HG23	2.10	0.51
2:C:156:GLU:OE2	2:C:176:ALA:HB3	2.10	0.51
3:F:7:SER:CB	3:F:8:PRO:CD	2.87	0.51
1:A:21:LEU:HD23	1:A:22:ILE:N	2.25	0.51
1:A:112:ILE:HG21	1:A:204:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:LEU:N	1:B:435:LEU:HD22	2.26	0.51
2:C:12:VAL:O	2:C:119:VAL:HA	2.10	0.51
3:F:7:SER:HB2	3:F:22:THR:HB	1.93	0.51
1:A:336:ILE:O	1:A:340:ARG:HG3	2.11	0.51
1:B:78:LEU:HA	1:B:81:VAL:HG22	1.93	0.51
1:B:457:GLU:O	1:B:458:ALA:CB	2.59	0.51
2:C:178:LEU:HB2	2:C:183:TYR:HE2	1.76	0.51
3:D:3:VAL:HB	3:D:26:SER:HB3	1.93	0.51
2:E:163:ASN:ND2	2:E:167:LEU:HD23	2.26	0.51
1:B:208:PHE:CD1	1:B:208:PHE:N	2.80	0.50
2:C:125:THR:HG22	2:C:126:PRO:O	2.11	0.50
3:D:32:ILE:HG22	3:D:33:HIS:N	2.27	0.50
1:B:201:ILE:O	1:B:201:ILE:HG13	2.11	0.50
3:D:6:GLN:HG3	3:D:100:GLY:H	1.76	0.50
3:D:184:GLU:O	3:D:187:ARG:HG2	2.11	0.50
2:E:30:SER:O	2:E:32:TYR:N	2.43	0.50
1:A:148:GLN:O	1:A:151:THR:N	2.35	0.50
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.47	0.50
3:D:77:MET:SD	3:D:103:LEU:HD21	2.50	0.50
3:F:73:THR:HG22	3:F:74:ILE:N	2.25	0.50
1:A:38:MET:HG3	1:A:168:LEU:CD2	2.40	0.50
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.75	0.50
1:B:419:TYR:CE1	1:B:422:ILE:HG21	2.47	0.50
3:D:189:ASN:ND2	3:D:211:ALA:H	2.05	0.50
1:A:71:THR:HB	1:A:77:LEU:CD2	2.41	0.50
1:A:79:LEU:H	1:A:79:LEU:CD2	2.23	0.50
1:B:143:MET:HG2	1:B:299:GLY:HA2	1.92	0.50
3:D:64:SER:OG	3:D:65:GLY:N	2.45	0.50
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.47	0.50
1:A:71:THR:HB	1:A:77:LEU:HD23	1.94	0.50
1:A:120:ARG:HD3	1:A:453:LEU:HD13	1.94	0.50
1:A:148:GLN:HG3	1:A:190:PHE:CZ	2.46	0.50
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.93	0.50
1:B:239:ILE:HG22	1:B:241:VAL:HG23	1.94	0.50
2:E:16:GLY:O	2:E:86:VAL:HG13	2.11	0.50
1:A:421:LEU:C	1:A:425:MET:HE2	2.31	0.50
1:B:71:THR:HB	1:B:77:LEU:CD2	2.41	0.50
1:B:287:ASN:HB3	1:B:290:LYS:HB2	1.94	0.50
2:C:49:GLY:HA3	2:C:70:ILE:HD12	1.94	0.50
3:D:7:SER:HB2	3:D:22:THR:HB	1.93	0.50
3:D:114:VAL:O	3:D:206:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196:TRP:O	2:E:197:PRO:C	2.48	0.50
1:A:423:LEU:O	1:A:427:ILE:HG13	2.11	0.50
1:B:166:PHE:O	1:B:168:LEU:N	2.44	0.50
1:B:200:ILE:O	1:B:200:ILE:CG2	2.60	0.50
1:B:272:TRP:N	1:B:272:TRP:CD1	2.78	0.50
1:B:320:ILE:N	1:B:321:PRO:CD	2.75	0.50
2:C:144:VAL:O	2:C:144:VAL:HG13	2.12	0.50
1:B:78:LEU:O	1:B:79:LEU:C	2.49	0.49
1:B:356:ILE:HG12	1:B:356:ILE:O	2.12	0.49
1:B:223:ILE:HG22	1:B:224:MET:N	2.25	0.49
1:B:421:LEU:O	1:B:425:MET:HG3	2.11	0.49
3:D:7:SER:CB	3:D:8:PRO:CD	2.89	0.49
2:E:64:LEU:N	2:E:64:LEU:HD23	2.27	0.49
2:E:185:LEU:HD12	2:E:185:LEU:C	2.32	0.49
1:A:18:ARG:HH11	1:B:457:GLU:HG2	1.76	0.49
1:A:255:TYR:HB3	1:A:428:THR:HG1	1.77	0.49
1:B:287:ASN:ND2	1:B:290:LYS:H	2.07	0.49
1:B:345:LEU:O	1:B:349:SER:N	2.36	0.49
1:B:411:LEU:O	1:B:411:LEU:HG	2.12	0.49
1:B:413:LEU:CD1	1:B:422:ILE:HD13	2.28	0.49
2:C:210:SER:OG	2:C:212:THR:HG23	2.12	0.49
3:D:73:THR:HG22	3:D:74:ILE:N	2.25	0.49
2:E:30:SER:C	2:E:32:TYR:N	2.65	0.49
2:E:163:ASN:O	2:E:164:SER:HB2	2.11	0.49
1:A:63:GLN:N	1:A:63:GLN:OE1	2.45	0.49
3:D:22:THR:HG22	3:D:23:CYS:H	1.75	0.49
3:F:153:GLU:HG3	3:F:154:ARG:N	2.28	0.49
1:A:358:ALA:HB3	1:A:359:PRO:CD	2.42	0.49
1:B:439:THR:O	1:B:439:THR:OG1	2.29	0.49
1:A:101:ALA:HB2	1:A:130:VAL:HG21	1.93	0.49
1:A:180:THR:OG1	1:A:181:GLY:N	2.46	0.49
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.95	0.49
1:B:139:LEU:HD13	1:B:147:ARG:HB3	1.94	0.49
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.47	0.49
2:C:131:PRO:HD3	2:C:216:LYS:HG2	1.94	0.49
3:F:114:VAL:HG22	3:F:135:LEU:CD2	2.42	0.49
1:B:422:ILE:O	1:B:426:ILE:HG13	2.13	0.49
1:A:116:LEU:HB3	1:A:206:PRO:HD3	1.94	0.49
1:A:172:GLU:O	1:A:176:THR:HB	2.13	0.49
1:A:320:ILE:N	1:A:321:PRO:CD	2.75	0.49
1:B:99:LYS:C	1:B:100:TYR:CD1	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:O	1:B:151:THR:N	2.36	0.49
1:B:367:LEU:HD12	1:B:367:LEU:O	2.12	0.49
1:B:398:LEU:HD22	1:B:402:ILE:HG21	1.95	0.49
2:C:196:TRP:HD1	2:C:201:VAL:HG23	1.77	0.49
2:E:51:ILE:HG23	2:E:51:ILE:O	2.12	0.49
1:A:148:GLN:HE21	1:A:189:ALA:HB1	1.77	0.49
1:B:35:ILE:O	1:B:38:MET:N	2.38	0.49
1:B:120:ARG:HD3	1:B:453:LEU:HD13	1.94	0.49
1:B:308:VAL:O	1:B:309:ALA:HB2	2.13	0.49
3:D:8:PRO:O	3:D:101:THR:HG23	2.12	0.49
3:D:153:GLU:O	3:D:154:ARG:HB2	2.12	0.49
2:E:45:LEU:HD11	3:F:86:TYR:CD1	2.48	0.49
1:B:267:PRO:HB3	1:B:441:GLY:CA	2.43	0.49
1:B:348:PHE:CD1	1:B:356:ILE:HB	2.48	0.49
2:C:132:LEU:CD2	3:D:132:VAL:HG21	2.37	0.49
2:E:38:ARG:HH21	2:E:46:LYS:HZ2	1.59	0.49
3:F:2:ILE:CD1	3:F:27:SER:HB2	2.38	0.49
3:F:113:THR:HG22	3:F:113:THR:O	2.12	0.49
3:F:114:VAL:HG12	3:F:115:SER:H	1.78	0.49
1:A:146:GLY:HA3	1:A:358:ALA:HB3	1.94	0.48
1:A:163:LEU:HD13	1:A:173:ALA:O	2.13	0.48
1:A:441:GLY:O	1:A:442:LYS:HG3	2.13	0.48
1:B:59:TRP:O	1:B:62:ASN:HB3	2.13	0.48
1:B:78:LEU:O	1:B:81:VAL:HG22	2.13	0.48
1:A:267:PRO:HB3	1:A:441:GLY:HA3	1.94	0.48
1:A:340:ARG:HA	1:A:343:THR:OG1	2.13	0.48
1:B:449:LEU:O	1:B:453:LEU:N	2.46	0.48
1:A:270:ASN:O	1:A:273:VAL:CG1	2.61	0.48
1:B:336:ILE:O	1:B:340:ARG:HG3	2.13	0.48
1:B:366:VAL:O	1:B:367:LEU:C	2.50	0.48
3:D:125:THR:HG22	3:D:125:THR:O	2.12	0.48
2:E:167:LEU:HD21	2:E:191:VAL:HG11	1.95	0.48
1:A:399:ALA:O	1:A:433:THR:HG23	2.13	0.48
1:B:360:MET:SD	1:B:397:LEU:HD13	2.53	0.48
2:C:124:THR:O	2:C:125:THR:OG1	2.23	0.48
1:A:131:LYS:HE3	1:A:150:PRO:HA	1.95	0.48
1:B:180:THR:OG1	1:B:181:GLY:N	2.46	0.48
1:B:383:HIS:CE1	3:F:90:TRP:CZ2	3.01	0.48
2:E:4:LEU:HB3	2:E:112:GLY:CA	2.44	0.48
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.44	0.48
1:A:360:MET:SD	1:A:397:LEU:HD12	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:HD13	1:A:444:LEU:C	2.33	0.48
1:A:457:GLU:O	1:A:459:GLU:N	2.46	0.48
1:B:198:LEU:CD1	1:B:406:LEU:HD23	2.44	0.48
1:B:401:SER:O	1:B:444:LEU:HB3	2.13	0.48
3:F:8:PRO:O	3:F:101:THR:HG23	2.12	0.48
1:A:398:LEU:O	1:A:402:ILE:CG2	2.62	0.48
1:B:273:VAL:HA	1:B:345:LEU:HD22	1.95	0.48
2:C:106:TRP:HD1	2:C:106:TRP:H	1.59	0.48
3:D:29:VAL:HG21	3:D:32:ILE:HD11	1.95	0.48
2:E:11:LEU:HB3	2:E:124:THR:CG2	2.43	0.48
3:F:65:GLY:CA	3:F:70:TYR:HA	2.44	0.48
3:F:115:SER:CB	3:F:117:PHE:HE1	2.27	0.48
1:B:171:ASP:HA	1:B:174:ARG:HH12	1.79	0.48
2:C:30:SER:C	2:C:32:TYR:N	2.66	0.48
2:C:32:TYR:CE2	2:C:98:ARG:HD3	2.49	0.48
1:A:160:ARG:HD2	1:A:163:LEU:HD23	1.96	0.48
1:A:459:GLU:O	1:A:459:GLU:HG2	2.13	0.48
1:B:342:ILE:O	1:B:344:THR:N	2.46	0.48
2:C:124:THR:CG2	2:C:125:THR:H	2.25	0.48
1:B:53:PHE:HA	1:B:132:PHE:HE2	1.79	0.48
3:D:93:HIS:CD2	3:D:94:PRO:HA	2.48	0.48
3:F:3:VAL:HB	3:F:26:SER:HB3	1.96	0.48
3:F:29:VAL:O	3:F:67:GLY:HA2	2.14	0.48
3:F:59:VAL:HG12	3:F:59:VAL:O	2.14	0.48
1:A:99:LYS:C	1:A:100:TYR:CD1	2.87	0.47
1:A:256:LEU:O	1:A:260:ILE:HG13	2.14	0.47
1:B:269:PHE:HE2	1:B:356:ILE:HD11	1.79	0.47
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.48	0.47
3:F:36:GLN:HG3	3:F:85:TYR:CE2	2.49	0.47
3:F:189:ASN:ND2	3:F:211:ALA:H	2.06	0.47
1:A:191:ASN:CG	1:A:191:ASN:O	2.53	0.47
1:A:201:ILE:O	1:A:201:ILE:HG13	2.14	0.47
3:D:110:ALA:C	3:D:199:THR:HG21	2.35	0.47
1:A:231:ILE:HB	1:A:232:PHE:CD1	2.49	0.47
1:A:53:PHE:HA	1:A:132:PHE:HE2	1.79	0.47
1:A:83:PHE:CD1	1:A:83:PHE:C	2.87	0.47
1:A:98:ARG:CZ	1:A:291:TRP:CZ3	2.98	0.47
1:A:358:ALA:N	4:A:474:BR:BR	2.91	0.47
1:B:318:ASN:C	1:B:318:ASN:ND2	2.67	0.47
3:D:89:GLN:CD	3:D:89:GLN:C	2.73	0.47
2:E:38:ARG:HE	2:E:46:LYS:NZ	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:LEU:HD23	2:E:96:CYS:HB2	1.96	0.47
2:E:178:LEU:HD12	2:E:182:LEU:O	2.15	0.47
1:B:250:ASN:ND2	1:B:382:TYR:CE2	2.83	0.47
1:A:78:LEU:O	1:A:81:VAL:N	2.48	0.47
1:B:180:THR:O	1:B:181:GLY:C	2.53	0.47
1:B:241:VAL:HG11	1:B:324:THR:HG21	1.96	0.47
2:C:70:ILE:HG12	2:C:81:LEU:HD13	1.96	0.47
1:B:60:LEU:O	1:B:64:ARG:HG3	2.14	0.47
1:B:155:GLY:HA3	1:B:181:GLY:O	2.15	0.47
1:B:163:LEU:CD2	1:B:174:ARG:HA	2.44	0.47
1:B:258:LEU:HG	1:B:258:LEU:O	2.14	0.47
2:C:24:ALA:HB1	2:C:27:PHE:CE1	2.49	0.47
3:D:127:GLY:HA2	3:D:182:LYS:HB2	1.96	0.47
1:B:160:ARG:O	1:B:163:LEU:N	2.48	0.47
2:C:170:GLY:O	2:C:189:VAL:HA	2.15	0.47
2:E:32:TYR:O	2:E:72:ARG:NH2	2.48	0.47
2:E:60:TYR:CD1	2:E:60:TYR:N	2.83	0.47
3:F:32:ILE:HG22	3:F:33:HIS:H	1.79	0.47
3:F:105:ILE:HD12	3:F:170:SER:OG	2.15	0.47
3:F:111:ALA:H	3:F:199:THR:HG21	1.79	0.47
1:A:232:PHE:CD1	1:A:232:PHE:N	2.83	0.47
1:A:358:ALA:O	1:A:360:MET:N	2.48	0.47
3:F:4:LEU:HD12	3:F:96:THR:O	2.15	0.47
3:F:22:THR:CG2	3:F:23:CYS:N	2.78	0.47
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.97	0.46
1:A:458:ALA:N	1:A:460:GLN:NE2	2.63	0.46
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.96	0.46
2:C:87:ARG:HG3	2:C:89:GLU:OE2	2.14	0.46
3:D:162:TRP:CD1	3:D:174:MET:HB2	2.50	0.46
2:E:49:GLY:HA3	2:E:70:ILE:HD11	1.97	0.46
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.50	0.46
1:A:176:THR:O	1:A:180:THR:HG23	2.16	0.46
1:A:398:LEU:CD2	1:A:402:ILE:HG21	2.45	0.46
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.50	0.46
3:F:127:GLY:O	3:F:182:LYS:N	2.42	0.46
1:B:387:GLY:O	1:B:390:ALA:N	2.45	0.46
2:E:87:ARG:HG3	2:E:89:GLU:OE2	2.15	0.46
3:F:89:GLN:C	3:F:89:GLN:CD	2.73	0.46
1:A:423:LEU:HB3	1:A:424:PRO:CD	2.34	0.46
1:B:122:VAL:O	1:B:124:TRP:N	2.45	0.46
1:B:356:ILE:O	1:B:360:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:86:TYR:CE2	3:D:100:GLY:HA3	2.50	0.46
1:A:155:GLY:HA3	1:A:181:GLY:O	2.15	0.46
1:A:320:ILE:CG2	1:A:394:MET:CE	2.91	0.46
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.51	0.46
3:F:6:GLN:HE21	3:F:6:GLN:HB3	1.51	0.46
3:F:82:ALA:HB2	3:F:105:ILE:CD1	2.39	0.46
3:F:153:GLU:O	3:F:154:ARG:HB2	2.14	0.46
1:B:126:ARG:O	1:B:130:VAL:HG23	2.16	0.46
1:B:444:LEU:HD13	1:B:444:LEU:C	2.36	0.46
2:C:72:ARG:O	2:C:72:ARG:HG2	2.16	0.46
3:D:153:GLU:HG3	3:D:154:ARG:N	2.30	0.46
3:F:54:THR:HG22	3:F:55:SER:N	2.30	0.46
1:A:108:GLY:CA	1:A:153:GLN:NE2	2.75	0.46
1:A:457:GLU:CG	1:A:458:ALA:N	2.70	0.46
3:D:185:TYR:HD1	3:D:191:TYR:CZ	2.34	0.46
1:A:143:MET:CE	1:A:347:CYS:SG	3.04	0.46
1:A:163:LEU:CD2	1:A:174:ARG:HA	2.45	0.46
1:B:74:ASN:O	1:B:77:LEU:HB3	2.16	0.46
1:B:91:MET:C	1:B:93:GLY:N	2.68	0.46
1:B:149:GLY:N	4:B:474:BR:BR	2.99	0.46
1:B:423:LEU:HG	1:B:427:ILE:CD1	2.46	0.46
2:C:189:VAL:O	2:C:189:VAL:CG1	2.59	0.46
2:E:69:ILE:HG22	2:E:69:ILE:O	2.15	0.46
1:A:78:LEU:O	1:A:81:VAL:HG22	2.16	0.46
1:B:44:THR:O	1:B:48:LEU:HD22	2.16	0.46
3:D:19:VAL:HG12	3:D:74:ILE:HB	1.97	0.46
2:E:134:PRO:HD3	2:E:146:LEU:CD2	2.46	0.46
1:A:333:LEU:O	1:A:336:ILE:N	2.49	0.46
1:B:38:MET:CG	1:B:168:LEU:HD21	2.43	0.46
1:B:131:LYS:HE3	1:B:150:PRO:HA	1.97	0.46
3:D:125:THR:O	3:D:126:SER:HB3	2.15	0.46
2:E:29:TYR:OH	2:E:34:MET:HG3	2.16	0.46
3:F:164:ASP:O	3:F:165:GLN:C	2.53	0.46
1:A:401:SER:O	1:A:444:LEU:CB	2.64	0.45
1:B:190:PHE:C	1:B:192:ALA:N	2.65	0.45
2:C:162:TRP:C	2:C:164:SER:N	2.70	0.45
3:D:29:VAL:HG23	3:D:70:TYR:CE1	2.50	0.45
3:F:184:GLU:O	3:F:187:ARG:HG2	2.16	0.45
1:A:208:PHE:CD1	1:A:208:PHE:N	2.84	0.45
1:A:279:LEU:HD23	1:A:279:LEU:O	2.17	0.45
1:B:309:ALA:H	1:B:310:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:PRO:O	1:B:445:ALA:N	2.49	0.45
2:C:121:SER:O	2:C:122:ALA:C	2.55	0.45
2:E:200:THR:HG22	2:E:200:THR:O	2.15	0.45
1:B:79:LEU:CD2	1:B:79:LEU:N	2.79	0.45
1:B:158:ILE:O	1:B:162:VAL:HG13	2.15	0.45
1:B:398:LEU:CD2	1:B:402:ILE:HG21	2.47	0.45
2:C:40:ALA:HB3	2:C:43:LYS:HB2	1.98	0.45
1:A:194:LEU:O	1:A:195:ALA:C	2.55	0.45
1:B:419:TYR:CG	1:B:419:TYR:O	2.69	0.45
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.46	0.45
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.51	0.45
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.52	0.45
1:A:399:ALA:HB1	1:A:405:PRO:HG3	1.99	0.45
1:B:98:ARG:H	1:B:98:ARG:HG2	1.47	0.45
1:B:124:TRP:CA	1:B:157:ASN:HD22	2.18	0.45
1:B:263:GLY:HA3	1:B:435:LEU:HB2	1.98	0.45
1:B:383:HIS:HE1	3:F:90:TRP:CZ2	2.34	0.45
3:D:33:HIS:CE1	3:D:49:ASP:H	2.35	0.45
3:F:7:SER:CB	3:F:22:THR:HB	2.47	0.45
3:F:75:ASN:O	3:F:76:THR:HB	2.16	0.45
1:A:98:ARG:H	1:A:98:ARG:HG2	1.38	0.45
1:A:214:SER:O	1:A:215:ILE:C	2.54	0.45
1:B:71:THR:HB	1:B:77:LEU:HD23	1.99	0.45
1:B:288:ILE:CG2	1:B:289:THR:N	2.80	0.45
1:B:360:MET:SD	1:B:397:LEU:CD1	3.05	0.45
2:E:99:LEU:HD21	2:E:108:PHE:CD2	2.52	0.45
3:F:114:VAL:HG13	3:F:135:LEU:CD2	2.47	0.45
3:F:178:LEU:HD12	3:F:179:THR:N	2.32	0.45
1:A:79:LEU:CD2	1:A:79:LEU:N	2.79	0.45
1:B:53:PHE:HE2	1:B:150:PRO:HB2	1.81	0.45
1:B:78:LEU:O	1:B:80:THR:N	2.49	0.45
1:B:218:VAL:O	1:B:222:VAL:HG23	2.17	0.45
1:B:421:LEU:O	1:B:424:PRO:HD2	2.16	0.45
2:C:66:ASP:O	2:C:67:LYS:C	2.53	0.45
2:C:67:LYS:HD3	2:C:67:LYS:HA	1.73	0.45
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.52	0.45
1:A:343:THR:O	1:A:347:CYS:HB2	2.17	0.45
1:B:92:PHE:O	1:B:92:PHE:CD1	2.70	0.45
2:C:185:LEU:C	2:C:185:LEU:CD1	2.85	0.45
3:D:7:SER:CB	3:D:22:THR:HB	2.46	0.45
3:D:32:ILE:HG12	3:D:70:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TRP:CZ3	3:D:87:CYS:HB3	2.52	0.45
1:A:78:LEU:O	1:A:80:THR:N	2.50	0.45
1:A:163:LEU:HA	1:A:168:LEU:HD11	1.98	0.45
1:A:287:ASN:ND2	1:A:290:LYS:H	2.14	0.45
1:B:160:ARG:HD2	1:B:163:LEU:HD23	1.99	0.45
1:B:167:ARG:HG2	1:B:167:ARG:HH11	1.82	0.45
1:B:182:ALA:HB1	1:B:204:MET:CE	2.40	0.45
2:C:18:LEU:N	2:C:18:LEU:CD2	2.80	0.45
2:C:111:TRP:CE3	3:D:43:PRO:HD2	2.52	0.45
2:C:152:GLY:HA2	2:C:182:LEU:HD13	1.98	0.45
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.51	0.45
1:A:148:GLN:O	1:A:149:GLY:C	2.55	0.45
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.99	0.45
1:A:411:LEU:O	1:A:414:GLU:HB2	2.17	0.45
1:B:78:LEU:O	1:B:81:VAL:N	2.50	0.45
1:B:148:GLN:HB2	4:B:474:BR:BR	2.72	0.45
1:B:294:MET:O	1:B:297:ALA:HB3	2.17	0.45
1:B:411:LEU:O	1:B:415:MET:HG2	2.17	0.45
2:C:167:LEU:HD21	2:C:191:VAL:HG11	1.99	0.45
3:F:50:THR:O	3:F:51:SER:HB3	2.17	0.45
3:F:115:SER:O	3:F:133:CYS:HA	2.17	0.45
1:A:200:ILE:HD11	1:A:204:MET:HE3	1.98	0.44
1:A:287:ASN:HB3	1:A:290:LYS:HB2	1.98	0.44
1:A:383:HIS:CD2	2:C:33:TRP:CZ3	3.01	0.44
1:B:63:GLN:N	1:B:63:GLN:OE1	2.49	0.44
3:D:29:VAL:O	3:D:67:GLY:HA2	2.17	0.44
2:E:67:LYS:HA	2:E:67:LYS:HD3	1.71	0.44
3:F:12:SER:HA	3:F:104:GLU:O	2.17	0.44
3:F:125:THR:O	3:F:125:THR:HG22	2.17	0.44
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.82	0.44
1:A:258:LEU:O	1:A:258:LEU:HG	2.16	0.44
1:A:284:HIS:CD2	1:A:291:TRP:CD2	3.06	0.44
1:A:324:THR:HG23	1:A:390:ALA:HB3	1.97	0.44
2:C:38:ARG:HH21	2:C:46:LYS:HZ2	1.64	0.44
2:C:174:PHE:CD1	3:D:163:THR:HG23	2.52	0.44
3:D:116:ILE:HD12	3:D:193:CYS:HB2	1.99	0.44
3:F:116:ILE:HD12	3:F:133:CYS:HB2	1.99	0.44
1:A:223:ILE:HD13	1:B:427:ILE:HG12	1.98	0.44
1:A:307:PHE:CG	1:A:307:PHE:O	2.70	0.44
1:A:340:ARG:HA	1:A:343:THR:HG1	1.82	0.44
1:A:406:LEU:HD21	1:B:198:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PHE:CG	1:B:307:PHE:O	2.70	0.44
2:C:38:ARG:HE	2:C:46:LYS:NZ	2.15	0.44
2:C:53:PRO:C	2:C:55:SER:H	2.20	0.44
3:D:93:HIS:CD2	3:D:94:PRO:CA	3.00	0.44
3:D:93:HIS:CG	3:D:94:PRO:HA	2.52	0.44
3:D:105:ILE:O	3:D:105:ILE:HG22	2.17	0.44
3:F:143:ILE:HG13	3:F:197:HIS:HB2	2.00	0.44
1:B:200:ILE:O	1:B:200:ILE:HG23	2.15	0.44
2:E:66:ASP:O	2:E:67:LYS:C	2.56	0.44
3:F:65:GLY:O	3:F:66:SER:HB3	2.17	0.44
3:F:125:THR:O	3:F:126:SER:HB3	2.17	0.44
2:C:51:ILE:HD11	2:C:55:SER:CB	2.43	0.44
1:A:27:GLU:OE2	1:A:30:LYS:CD	2.65	0.44
1:A:308:VAL:O	1:A:309:ALA:CB	2.66	0.44
2:E:18:LEU:N	2:E:18:LEU:CD2	2.81	0.44
2:E:170:GLY:O	2:E:189:VAL:HA	2.17	0.44
1:A:45:LEU:N	1:A:45:LEU:HD12	2.32	0.44
1:A:262:PHE:O	1:A:266:GLY:N	2.49	0.44
1:A:269:PHE:HE2	1:A:356:ILE:HD11	1.82	0.44
1:B:83:PHE:CD1	1:B:83:PHE:C	2.90	0.44
3:F:64:SER:OG	3:F:65:GLY:N	2.50	0.44
1:A:273:VAL:HA	1:A:345:LEU:HD22	1.99	0.44
2:C:210:SER:O	2:C:212:THR:HG23	2.17	0.44
2:E:150:VAL:HB	2:E:185:LEU:HD12	2.00	0.44
1:A:415:MET:O	1:A:416:THR:HG22	2.17	0.44
1:B:94:TYR:OH	1:B:352:ALA:HB2	2.18	0.44
1:B:252:LEU:O	1:B:253:TRP:C	2.55	0.44
2:C:38:ARG:HE	2:C:46:LYS:HE3	1.82	0.44
3:D:60:ARG:NH1	3:D:81:ASP:OD1	2.51	0.44
3:F:93:HIS:CG	3:F:94:PRO:HA	2.53	0.44
3:F:192:THR:CB	3:F:207:SER:HB3	2.48	0.44
1:B:135:GLY:O	1:B:136:LEU:C	2.55	0.43
1:B:427:ILE:HG22	1:B:427:ILE:O	2.18	0.43
2:E:181:ALA:O	2:E:182:LEU:HD23	2.17	0.43
3:F:107:ARG:NE	3:F:108:ALA:O	2.51	0.43
1:A:250:ASN:ND2	2:C:105:TYR:CE1	2.78	0.43
1:B:143:MET:CE	1:B:347:CYS:SG	3.06	0.43
2:C:72:ARG:HG3	2:C:74:ASN:OD1	2.18	0.43
2:C:126:PRO:HA	2:C:210:SER:CB	2.48	0.43
3:D:22:THR:CG2	3:D:23:CYS:N	2.80	0.43
2:E:18:LEU:HD11	2:E:117:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:O	1:A:186:LEU:HG	2.18	0.43
1:B:48:LEU:HD22	1:B:48:LEU:N	2.22	0.43
1:B:342:ILE:HG22	1:B:343:THR:N	2.34	0.43
1:B:398:LEU:HD23	1:B:398:LEU:HA	1.87	0.43
2:E:171:VAL:C	2:E:172:HIS:HD1	2.21	0.43
1:B:320:ILE:CG2	1:B:394:MET:CE	2.91	0.43
1:B:441:GLY:O	1:B:442:LYS:CG	2.65	0.43
2:C:39:GLN:C	2:C:92:ALA:HB1	2.38	0.43
3:F:119:PRO:HD3	3:F:131:VAL:HG22	2.00	0.43
1:A:234:HIS:O	1:A:236:VAL:N	2.49	0.43
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.85	0.43
1:B:443:PRO:C	1:B:445:ALA:N	2.72	0.43
2:C:2:VAL:O	2:C:2:VAL:CG1	2.66	0.43
2:C:146:LEU:HD13	2:C:218:ILE:HG21	2.00	0.43
3:D:74:ILE:CG2	3:D:77:MET:HA	2.48	0.43
3:F:32:ILE:CG2	3:F:33:HIS:N	2.80	0.43
3:F:86:TYR:HE2	3:F:100:GLY:HA3	1.84	0.43
1:A:32:PRO:HD2	1:A:35:ILE:HD12	2.01	0.43
1:B:53:PHE:CE2	1:B:150:PRO:HB2	2.54	0.43
1:B:423:LEU:O	1:B:427:ILE:HG13	2.19	0.43
2:C:61:THR:OG1	2:C:62:PRO:HD2	2.18	0.43
2:E:162:TRP:CZ3	2:E:203:CYS:CB	3.01	0.43
1:A:33:LEU:C	1:A:33:LEU:HD23	2.39	0.43
1:A:220:ILE:HG12	1:B:430:LEU:CD2	2.49	0.43
1:A:366:VAL:O	1:A:367:LEU:C	2.53	0.43
1:B:71:THR:OG1	1:B:78:LEU:HD23	2.19	0.43
1:B:305:LEU:O	1:B:307:PHE:N	2.52	0.43
2:C:69:ILE:HB	2:C:82:GLN:HB2	2.01	0.43
2:C:196:TRP:HD1	2:C:201:VAL:CG2	2.32	0.43
2:E:27:PHE:HE2	2:E:98:ARG:HG3	1.83	0.43
3:F:60:ARG:HD3	3:F:78:GLU:HG2	1.99	0.43
1:A:200:ILE:HG23	1:A:200:ILE:O	2.19	0.43
1:B:262:PHE:O	1:B:266:GLY:N	2.52	0.43
1:B:397:LEU:O	1:B:401:SER:HB2	2.19	0.43
2:C:172:HIS:CB	2:C:188:SER:HB3	2.39	0.43
3:D:124:LEU:O	3:D:182:LYS:HD2	2.19	0.43
3:F:185:TYR:HD1	3:F:191:TYR:HH	1.65	0.43
1:B:91:MET:O	1:B:92:PHE:C	2.56	0.43
1:B:136:LEU:HD12	1:B:136:LEU:H	1.84	0.43
1:B:295:GLY:C	1:B:297:ALA:N	2.71	0.43
2:E:40:ALA:HB3	2:E:43:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.37	0.43
2:E:176:ALA:HA	2:E:185:LEU:HB3	2.01	0.43
3:F:79:ALA:CA	3:F:105:ILE:HD13	2.48	0.43
3:F:127:GLY:HA2	3:F:182:LYS:HB2	2.00	0.43
1:A:83:PHE:HB2	1:A:304:LEU:HD13	2.01	0.43
1:A:117:GLU:CD	1:A:206:PRO:HB3	2.40	0.43
1:B:95:PHE:C	1:B:97:VAL:H	2.22	0.43
3:D:164:ASP:O	3:D:165:GLN:C	2.56	0.43
2:E:156:GLU:OE2	2:E:176:ALA:HB3	2.18	0.43
3:F:58:PRO:C	3:F:60:ARG:N	2.71	0.43
1:A:287:ASN:ND2	1:A:289:THR:HB	2.34	0.42
1:A:309:ALA:N	1:A:310:PRO:HD3	2.33	0.42
1:B:144:VAL:HG21	1:B:343:THR:CB	2.43	0.42
1:B:169:LYS:CG	1:B:170:GLY:N	2.81	0.42
1:B:200:ILE:HA	1:B:204:MET:HB2	2.01	0.42
1:B:256:LEU:O	1:B:260:ILE:HG13	2.19	0.42
1:B:271:LYS:O	1:B:272:TRP:C	2.57	0.42
2:C:6:GLU:CD	2:C:114:GLY:HA2	2.40	0.42
2:C:61:THR:OG1	2:C:62:PRO:CD	2.67	0.42
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.54	0.42
2:E:106:TRP:CD1	2:E:106:TRP:N	2.79	0.42
1:A:305:LEU:C	1:A:307:PHE:N	2.70	0.42
1:B:23:ARG:HG3	1:B:23:ARG:NH1	2.34	0.42
2:C:111:TRP:N	2:C:111:TRP:CD1	2.87	0.42
2:E:38:ARG:HE	2:E:46:LYS:HE3	1.84	0.42
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.77	0.42
1:A:139:LEU:O	1:A:142:GLY:N	2.52	0.42
1:B:68:LEU:HD22	1:B:78:LEU:HD22	2.01	0.42
1:B:128:LEU:HB2	1:B:129:PRO:HD3	2.01	0.42
1:B:336:ILE:O	1:B:336:ILE:HG22	2.19	0.42
1:A:200:ILE:O	1:A:200:ILE:CG2	2.66	0.42
1:A:387:GLY:O	1:A:390:ALA:N	2.48	0.42
1:B:153:GLN:C	1:B:155:GLY:N	2.69	0.42
1:B:172:GLU:O	1:B:176:THR:HB	2.19	0.42
1:B:227:ILE:HD12	1:B:227:ILE:N	2.35	0.42
1:B:331:GLY:O	1:B:332:MET:C	2.56	0.42
1:B:431:GLY:O	1:B:432:ALA:O	2.37	0.42
1:B:447:ALA:O	1:B:450:ALA:HB3	2.19	0.42
3:D:76:THR:HG22	3:D:76:THR:O	2.18	0.42
2:E:4:LEU:HB3	2:E:112:GLY:HA2	2.02	0.42
2:E:72:ARG:HG3	2:E:74:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TYR:O	1:A:78:LEU:N	2.52	0.42
1:A:205:ARG:O	1:A:206:PRO:C	2.57	0.42
1:B:81:VAL:HG23	1:B:82:ALA:N	2.35	0.42
1:B:92:PHE:CD1	1:B:92:PHE:C	2.93	0.42
1:B:250:ASN:ND2	2:E:105:TYR:CD1	2.87	0.42
3:F:118:PRO:O	3:F:119:PRO:C	2.58	0.42
1:A:108:GLY:CA	1:A:153:GLN:HE21	2.31	0.42
1:A:143:MET:HE2	1:A:347:CYS:SG	2.60	0.42
1:A:166:PHE:C	1:A:168:LEU:H	2.22	0.42
1:A:193:PRO:HG2	1:A:194:LEU:H	1.84	0.42
1:A:198:LEU:CD1	1:A:406:LEU:HD23	2.48	0.42
1:A:305:LEU:O	1:A:307:PHE:N	2.52	0.42
1:A:317:PHE:HD2	1:A:317:PHE:HA	1.75	0.42
1:A:443:PRO:O	1:A:446:SER:N	2.52	0.42
1:B:138:THR:OG1	1:B:353:PRO:HG2	2.20	0.42
1:B:200:ILE:HD11	1:B:204:MET:HE3	2.01	0.42
1:B:413:LEU:O	1:B:413:LEU:HD23	2.19	0.42
2:E:18:LEU:HD11	2:E:117:VAL:CG2	2.50	0.42
1:A:91:MET:HG3	1:A:296:GLY:HA3	2.00	0.42
1:A:180:THR:O	1:A:184:ALA:N	2.29	0.42
1:A:284:HIS:C	1:A:286:GLY:N	2.73	0.42
1:A:427:ILE:O	1:A:427:ILE:HG22	2.19	0.42
1:A:435:LEU:N	1:A:435:LEU:HD22	2.35	0.42
1:B:331:GLY:C	1:B:333:LEU:N	2.72	0.42
2:E:5:LEU:HD13	2:E:5:LEU:C	2.39	0.42
3:F:79:ALA:C	3:F:81:ASP:H	2.22	0.42
3:F:187:ARG:HG3	3:F:187:ARG:O	2.20	0.42
1:B:81:VAL:C	1:B:83:PHE:H	2.23	0.42
1:B:91:MET:HG3	1:B:296:GLY:HA3	2.02	0.42
1:B:111:GLU:O	1:B:114:GLY:N	2.53	0.42
2:C:8:GLY:O	2:C:9:GLY:O	2.38	0.42
2:C:126:PRO:CB	2:C:210:SER:OG	2.65	0.42
3:D:35:TYR:HE1	3:D:88:GLN:HB3	1.84	0.42
3:D:105:ILE:HB	3:D:170:SER:OG	2.19	0.42
3:F:73:THR:CG2	3:F:74:ILE:N	2.82	0.42
1:A:360:MET:SD	1:A:397:LEU:HD13	2.60	0.42
1:A:380:PRO:CD	1:A:381:GLN:NE2	2.79	0.42
1:B:270:ASN:O	1:B:271:LYS:C	2.57	0.42
1:B:443:PRO:O	1:B:446:SER:N	2.52	0.42
3:D:47:ILE:HG22	3:D:48:TYR:N	2.35	0.42
3:F:86:TYR:CE2	3:F:100:GLY:HA3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:O	1:B:437:GLN:HG3	2.20	0.42
1:A:68:LEU:HD22	1:A:78:LEU:HD22	2.01	0.42
1:A:267:PRO:HB3	1:A:441:GLY:CA	2.50	0.42
1:A:294:MET:O	1:A:297:ALA:HB3	2.19	0.42
1:A:385:GLU:O	1:A:386:ALA:C	2.57	0.42
1:A:413:LEU:HD23	1:A:413:LEU:O	2.20	0.42
1:B:279:LEU:HD23	1:B:279:LEU:C	2.39	0.42
1:B:398:LEU:O	1:B:402:ILE:CG2	2.68	0.42
1:B:418:ASN:C	1:B:420:GLN:H	2.24	0.42
2:C:196:TRP:CG	2:C:197:PRO:N	2.88	0.42
3:D:201:THR:HG23	3:D:202:SER:N	2.35	0.42
1:A:250:ASN:ND2	2:C:105:TYR:CD1	2.88	0.41
1:B:116:LEU:HB3	1:B:206:PRO:HD3	2.02	0.41
1:B:139:LEU:O	1:B:142:GLY:N	2.52	0.41
1:B:331:GLY:O	1:B:334:VAL:N	2.53	0.41
1:B:449:LEU:O	1:B:453:LEU:HB2	2.20	0.41
2:C:4:LEU:HD12	2:C:4:LEU:HA	1.79	0.41
3:F:33:HIS:CE1	3:F:49:ASP:H	2.38	0.41
1:A:284:HIS:NE2	1:A:291:TRP:CD2	2.88	0.41
1:A:443:PRO:C	1:A:445:ALA:N	2.73	0.41
1:B:111:GLU:O	1:B:112:ILE:C	2.59	0.41
1:B:120:ARG:HA	1:B:121:PRO:HD3	1.82	0.41
1:B:176:THR:HG22	1:B:177:LEU:HD23	2.01	0.41
3:D:74:ILE:HG21	3:D:77:MET:HA	2.02	0.41
2:E:11:LEU:HD23	2:E:124:THR:HG23	2.02	0.41
3:F:60:ARG:NH1	3:F:81:ASP:OD1	2.54	0.41
1:A:233:ASN:O	1:A:234:HIS:O	2.38	0.41
1:A:247:ALA:HA	1:A:248:PRO:HD2	1.75	0.41
1:B:212:LEU:N	1:B:212:LEU:CD1	2.82	0.41
1:B:413:LEU:HD12	1:B:422:ILE:CD1	2.29	0.41
2:C:107:TYR:HB3	3:D:33:HIS:NE2	2.34	0.41
2:C:171:VAL:C	2:C:172:HIS:HD1	2.24	0.41
3:D:58:PRO:C	3:D:60:ARG:N	2.74	0.41
1:A:180:THR:C	1:A:182:ALA:N	2.73	0.41
1:A:437:GLN:C	1:A:439:THR:H	2.23	0.41
1:B:247:ALA:HA	1:B:248:PRO:HD2	1.72	0.41
1:B:305:LEU:C	1:B:307:PHE:N	2.73	0.41
2:C:109:ASP:CG	2:C:110:VAL:HG23	2.39	0.41
2:C:151:LYS:HE3	2:C:151:LYS:HB2	1.84	0.41
3:D:79:ALA:C	3:D:81:ASP:H	2.23	0.41
3:F:181:THR:O	3:F:182:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:185:TYR:HD1	3:F:191:TYR:CZ	2.39	0.41
1:B:148:GLN:NE2	1:B:189:ALA:HB1	2.35	0.41
1:B:194:LEU:N	1:B:414:GLU:OE2	2.53	0.41
1:B:422:ILE:HA	1:B:425:MET:HE3	2.03	0.41
2:C:165:GLY:C	2:C:167:LEU:H	2.24	0.41
3:D:44:LYS:HE2	3:D:44:LYS:HB2	1.83	0.41
2:E:53:PRO:C	2:E:55:SER:H	2.24	0.41
1:A:169:LYS:CG	1:A:170:GLY:N	2.83	0.41
1:A:279:LEU:HD23	1:A:279:LEU:C	2.40	0.41
1:B:31:THR:HA	1:B:32:PRO:HD3	1.89	0.41
1:B:144:VAL:HB	1:B:343:THR:O	2.19	0.41
1:B:153:GLN:O	1:B:155:GLY:N	2.53	0.41
1:B:410:ILE:O	1:B:410:ILE:HG22	2.20	0.41
1:B:440:GLY:O	1:B:441:GLY:O	2.38	0.41
2:C:134:PRO:HD3	2:C:146:LEU:CD2	2.51	0.41
2:E:29:TYR:CZ	2:E:34:MET:HG3	2.56	0.41
2:E:72:ARG:O	2:E:72:ARG:HG2	2.21	0.41
1:A:64:ARG:HB3	1:A:64:ARG:NH1	2.35	0.41
1:A:295:GLY:C	1:A:297:ALA:N	2.72	0.41
1:B:114:GLY:C	1:B:116:LEU:N	2.74	0.41
1:B:284:HIS:CD2	1:B:291:TRP:CD2	3.08	0.41
2:E:118:THR:OG1	2:E:155:PRO:HG3	2.20	0.41
1:A:94:TYR:O	1:A:98:ARG:HG2	2.20	0.41
1:A:117:GLU:O	1:A:118:ASP:HB2	2.21	0.41
1:A:276:MET:O	1:A:280:LEU:HB2	2.21	0.41
1:B:65:MET:O	1:B:67:ALA:N	2.54	0.41
1:B:83:PHE:HB2	1:B:304:LEU:HD13	2.03	0.41
1:B:260:ILE:HG13	1:B:260:ILE:H	1.70	0.41
2:C:51:ILE:HG13	2:C:58:ILE:HG12	2.01	0.41
2:C:144:VAL:HG12	2:C:191:VAL:O	2.21	0.41
3:D:105:ILE:HD12	3:D:170:SER:OG	2.21	0.41
1:A:65:MET:O	1:A:67:ALA:N	2.54	0.41
1:A:81:VAL:C	1:A:83:PHE:H	2.23	0.41
1:A:128:LEU:CB	1:A:129:PRO:CD	2.98	0.41
1:A:272:TRP:N	1:A:272:TRP:CD1	2.87	0.41
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.87	0.41
1:A:441:GLY:O	1:A:442:LYS:CG	2.67	0.41
1:B:48:LEU:H	1:B:48:LEU:CD2	2.20	0.41
1:B:338:VAL:O	1:B:339:ALA:C	2.59	0.41
2:C:32:TYR:O	2:C:72:ARG:NH2	2.54	0.41
2:C:64:LEU:N	2:C:64:LEU:HD23	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:LEU:HD11	2:C:196:TRP:CD1	2.56	0.41
3:D:75:ASN:O	3:D:76:THR:HB	2.21	0.41
2:E:32:TYR:CE2	2:E:98:ARG:HD3	2.56	0.41
2:E:37:VAL:HG22	2:E:47:TRP:HA	2.01	0.41
2:E:126:PRO:HB3	2:E:210:SER:HG	1.85	0.41
3:F:6:GLN:HG3	3:F:99:GLY:N	2.35	0.41
3:F:124:LEU:O	3:F:182:LYS:HD2	2.21	0.41
1:A:101:ALA:CB	1:A:130:VAL:HG21	2.50	0.41
1:B:212:LEU:H	1:B:212:LEU:CD1	2.33	0.41
1:B:312:THR:HG22	1:B:339:ALA:HB3	2.02	0.41
3:F:115:SER:CB	3:F:117:PHE:CE1	3.03	0.41
3:F:189:ASN:ND2	3:F:210:ARG:N	2.69	0.41
1:B:94:TYR:O	1:B:98:ARG:HG2	2.20	0.40
2:C:165:GLY:C	2:C:167:LEU:N	2.73	0.40
3:D:201:THR:CG2	3:D:202:SER:N	2.84	0.40
2:E:196:TRP:HD1	2:E:201:VAL:HG23	1.86	0.40
3:F:46:TRP:HA	3:F:46:TRP:CE3	2.56	0.40
3:F:202:SER:HA	3:F:203:PRO:HD2	1.93	0.40
1:A:190:PHE:C	1:A:192:ALA:N	2.72	0.40
1:A:387:GLY:O	1:A:390:ALA:HB3	2.20	0.40
1:B:163:LEU:HA	1:B:168:LEU:HD11	2.02	0.40
1:B:309:ALA:N	1:B:310:PRO:HD3	2.36	0.40
1:B:342:ILE:C	1:B:344:THR:N	2.75	0.40
1:B:382:TYR:HB3	1:B:384:LEU:CD2	2.49	0.40
1:B:431:GLY:O	1:B:432:ALA:C	2.59	0.40
2:C:29:TYR:OH	2:C:34:MET:HG3	2.21	0.40
2:C:107:TYR:C	2:C:107:TYR:CD1	2.94	0.40
2:C:158:VAL:CG2	2:C:185:LEU:HD21	2.51	0.40
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.57	0.40
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.88	0.40
1:A:75:TYR:O	1:A:77:LEU:N	2.54	0.40
1:A:92:PHE:O	1:A:92:PHE:CD1	2.74	0.40
1:A:143:MET:HG2	1:A:299:GLY:HA2	2.02	0.40
1:A:179:ALA:O	1:A:200:ILE:HG12	2.21	0.40
1:B:128:LEU:CB	1:B:129:PRO:CD	2.99	0.40
1:B:288:ILE:HG23	1:B:289:THR:N	2.36	0.40
2:C:163:ASN:O	2:C:164:SER:HB2	2.21	0.40
2:C:207:HIS:CE1	2:C:210:SER:H	2.39	0.40
3:D:50:THR:O	3:D:51:SER:CB	2.64	0.40
3:D:185:TYR:CE1	3:D:191:TYR:CE1	3.09	0.40
2:E:104:GLY:O	2:E:106:TRP:HD1	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.89	0.40
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.93	0.40
3:D:73:THR:CG2	3:D:74:ILE:N	2.85	0.40
3:D:192:THR:CB	3:D:207:SER:HB3	2.52	0.40
2:E:72:ARG:HG3	2:E:72:ARG:HH11	1.85	0.40
2:E:196:TRP:CG	2:E:197:PRO:N	2.88	0.40
1:A:92:PHE:CD1	1:A:92:PHE:C	2.95	0.40
1:A:139:LEU:CD1	1:A:147:ARG:HB3	2.51	0.40
1:B:95:PHE:O	1:B:97:VAL:N	2.55	0.40
1:B:148:GLN:O	1:B:149:GLY:C	2.60	0.40
2:C:51:ILE:O	2:C:51:ILE:HG23	2.22	0.40
2:E:131:PRO:HD3	2:E:216:LYS:HG2	2.04	0.40
3:F:12:SER:OG	3:F:104:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/473 (93%)	305 (69%)	108 (24%)	29 (7%)	1	16
1	B	439/473 (93%)	294 (67%)	116 (26%)	29 (7%)	1	16
2	C	219/222 (99%)	179 (82%)	26 (12%)	14 (6%)	1	16
2	E	219/222 (99%)	175 (80%)	31 (14%)	13 (6%)	1	17
3	D	209/211 (99%)	173 (83%)	25 (12%)	11 (5%)	2	19
3	F	209/211 (99%)	164 (78%)	33 (16%)	12 (6%)	1	18
All	All	1737/1812 (96%)	1290 (74%)	339 (20%)	108 (6%)	1	17

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
1	A	234	HIS
1	A	309	ALA
1	B	167	ARG
1	B	191	ASN
1	B	234	HIS
1	B	309	ALA
2	C	65	LYS
2	C	106	TRP
2	C	140	ALA
3	D	7	SER
3	D	51	SER
3	D	67	GLY
3	D	126	SER
2	E	65	LYS
2	E	106	TRP
2	E	122	ALA
2	E	140	ALA
3	F	7	SER
3	F	112	PRO
3	F	126	SER
1	A	285	GLY
1	A	419	TYR
1	A	432	ALA
1	A	441	GLY
1	B	132	PHE
1	B	285	GLY
1	B	332	MET
1	B	343	THR
1	B	419	TYR
1	B	432	ALA
1	B	441	GLY
2	C	9	GLY
2	C	122	ALA
3	D	105	ILE
3	D	153	GLU
2	E	9	GLY
3	F	51	SER
3	F	67	GLY
3	F	153	GLU
1	A	78	LEU
1	A	132	PHE
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	318	ASN
1	B	78	LEU
1	B	223	ILE
1	B	318	ASN
1	B	444	LEU
2	C	31	ARG
2	C	109	ASP
2	C	196	TRP
3	D	55	SER
3	D	154	ARG
2	E	64	LEU
3	F	15	PRO
3	F	113	THR
3	F	154	ARG
1	A	79	LEU
1	A	223	ILE
1	A	235	GLU
1	A	274	LEU
1	A	332	MET
1	A	337	PHE
1	A	458	ALA
1	B	79	LEU
1	B	96	LEU
1	B	121	PRO
1	B	128	LEU
1	B	171	ASP
1	B	204	MET
1	B	206	PRO
1	B	274	LEU
1	B	306	GLY
1	B	443	PRO
2	C	53	PRO
3	D	15	PRO
3	D	199	THR
2	E	31	ARG
2	E	53	PRO
2	E	196	TRP
3	F	66	SER
1	A	137	GLY
1	A	171	ASP
1	A	206	PRO
1	A	215	ILE

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Mol	Chain	Res	Type
1	A	343	THR
1	A	438	PHE
1	A	443	PRO
2	C	124	THR
3	D	80	GLU
2	E	113	ALA
1	A	359	PRO
2	C	166	SER
3	F	55	SER
1	A	128	LEU
1	A	306	GLY
2	C	62	PRO
1	A	310	PRO
1	B	215	ILE
2	C	54	VAL
2	E	14	PRO
3	F	119	PRO
1	B	366	VAL
1	B	130	VAL
1	B	359	PRO
2	E	69	ILE
2	C	157	PRO
2	E	157	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	333/356 (94%)	302 (91%)	31 (9%)	9	37
1	B	330/356 (93%)	301 (91%)	29 (9%)	10	39
2	C	181/182 (100%)	160 (88%)	21 (12%)	5	29
2	E	181/182 (100%)	162 (90%)	19 (10%)	7	32
3	D	185/185 (100%)	177 (96%)	8 (4%)	29	63
3	F	185/185 (100%)	174 (94%)	11 (6%)	19	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1395/1446 (96%)	1276 (92%)	119 (8%)	10	40

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	63	GLN
1	A	73	ASP
1	A	79	LEU
1	A	98	ARG
1	A	103	GLU
1	A	120	ARG
1	A	167	ARG
1	A	168	LEU
1	A	176	THR
1	A	201	ILE
1	A	204	MET
1	A	206	PRO
1	A	207	GLN
1	A	208	PHE
1	A	211	THR
1	A	212	LEU
1	A	230	ARG
1	A	246	ASP
1	A	274	LEU
1	A	317	PHE
1	A	318	ASN
1	A	340	ARG
1	A	347	CYS
1	A	363	LEU
1	A	379	PHE
1	A	381	GLN
1	A	397	LEU
1	A	420	GLN
1	A	434	LEU
1	A	451	ARG
1	B	62	ASN
1	B	63	GLN
1	B	73	ASP
1	B	79	LEU
1	B	98	ARG
1	B	103	GLU

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Mol	Chain	Res	Type
1	B	120	ARG
1	B	150	PRO
1	B	167	ARG
1	B	168	LEU
1	B	201	ILE
1	B	207	GLN
1	B	208	PHE
1	B	212	LEU
1	B	230	ARG
1	B	246	ASP
1	B	274	LEU
1	B	317	PHE
1	B	318	ASN
1	B	340	ARG
1	B	347	CYS
1	B	363	LEU
1	B	379	PHE
1	B	381	GLN
1	B	397	LEU
1	B	418	ASN
1	B	420	GLN
1	B	434	LEU
1	B	451	ARG
2	C	4	LEU
2	C	18	LEU
2	C	27	PHE
2	C	45	LEU
2	C	59	ASN
2	C	67	LYS
2	C	72	ARG
2	C	77	ASP
2	C	98	ARG
2	C	107	TYR
2	C	115	THR
2	C	128	SER
2	C	155	PRO
2	C	157	PRO
2	C	167	LEU
2	C	172	HIS
2	C	186	SER
2	C	200	THR
2	C	203	CYS

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Mol	Chain	Res	Type
2	C	204	ASN
2	C	221	ARG
3	D	28	SER
3	D	46	TRP
3	D	75	ASN
3	D	77	MET
3	D	88	GLN
3	D	117	PHE
3	D	146	LYS
3	D	189	ASN
2	E	4	LEU
2	E	22	CYS
2	E	27	PHE
2	E	45	LEU
2	E	59	ASN
2	E	61	THR
2	E	67	LYS
2	E	72	ARG
2	E	77	ASP
2	E	98	ARG
2	E	107	TYR
2	E	121	SER
2	E	124	THR
2	E	157	PRO
2	E	167	LEU
2	E	172	HIS
2	E	200	THR
2	E	203	CYS
2	E	204	ASN
3	F	1	ASP
3	F	6	GLN
3	F	28	SER
3	F	46	TRP
3	F	75	ASN
3	F	77	MET
3	F	88	GLN
3	F	102	LYS
3	F	119	PRO
3	F	146	LYS
3	F	189	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	148	GLN
1	A	157	ASN
1	A	233	ASN
1	A	270	ASN
1	A	287	ASN
1	A	318	ASN
1	A	327	ASN
1	A	381	GLN
1	A	383	HIS
1	A	420	GLN
1	A	456	GLN
1	A	460	GLN
1	B	62	ASN
1	B	148	GLN
1	B	157	ASN
1	B	233	ASN
1	B	270	ASN
1	B	287	ASN
1	B	318	ASN
1	B	327	ASN
1	B	381	GLN
1	B	383	HIS
1	B	420	GLN
1	B	456	GLN
2	C	163	ASN
3	D	93	HIS
3	D	136	ASN
3	D	137	ASN
3	D	155	GLN
3	D	189	ASN
2	E	163	ASN
3	F	136	ASN
3	F	155	GLN
3	F	189	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	F	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	107:ARG	C	108:ALA	N	1.62
1	C	121:SER	C	122:ALA	N	1.18

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.67	3 (0%) 87 79	31, 86, 158, 204	0
1	B	441/473 (93%)	-0.71	3 (0%) 87 79	25, 73, 148, 205	0
2	C	221/222 (99%)	-0.46	4 (1%) 68 54	31, 77, 157, 205	0
2	E	221/222 (99%)	-0.32	1 (0%) 91 84	31, 92, 169, 198	0
3	D	211/211 (100%)	-0.32	1 (0%) 91 84	41, 104, 162, 204	0
3	F	211/211 (100%)	-0.38	0 100 100	29, 81, 145, 172	0
All	All	1749/1812 (96%)	-0.53	12 (0%) 87 79	25, 83, 161, 205	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	GLU	4.9
2	C	137	ALA	3.9
1	A	235	GLU	3.8
1	B	236	VAL	3.2
2	C	136	SER	3.0
2	C	140	ALA	2.9
2	C	139	ALA	2.6
1	B	234	HIS	2.5
3	D	127	GLY	2.4
1	A	29	ASP	2.2
1	A	234	HIS	2.2
2	E	43	LYS	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BR	B	474	1/1	0.89	0.23	138,138,138,138	0
4	BR	A	474	1/1	0.90	0.07	124,124,124,124	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.