



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:58 AM GMT

PDB ID : 2EXW
Title : Crystal structure of a EcClC-Fab complex in the absence of bound ions
Authors : Lobet, S.; Dutzler, R.
Deposited on : 2005-11-09
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

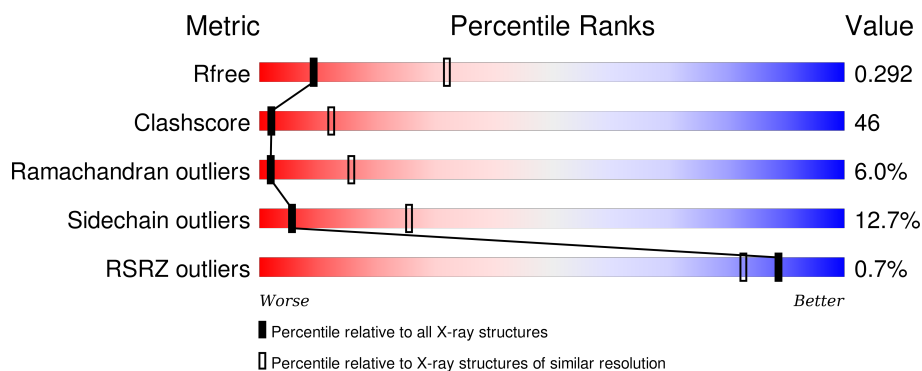
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>42%</div> <div>46%</div> <div>5%</div> <div>6%</div> </div>
1	B	473	<div> <div>42%</div> <div>45%</div> <div>6%</div> <div>7%</div> </div>
2	C	222	<div> <div>%</div> <div>36%</div> <div>47%</div> <div>14%</div> <div>•</div> </div>
2	E	222	<div> <div>%</div> <div>31%</div> <div>50%</div> <div>17%</div> <div>•</div> </div>
3	D	211	<div> <div>29%</div> <div>54%</div> <div>16%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	211	<div><div><div>%</div><div><div></div><div>28%</div><div>55%</div><div>15%</div><div></div></div><div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13223 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
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

- 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			

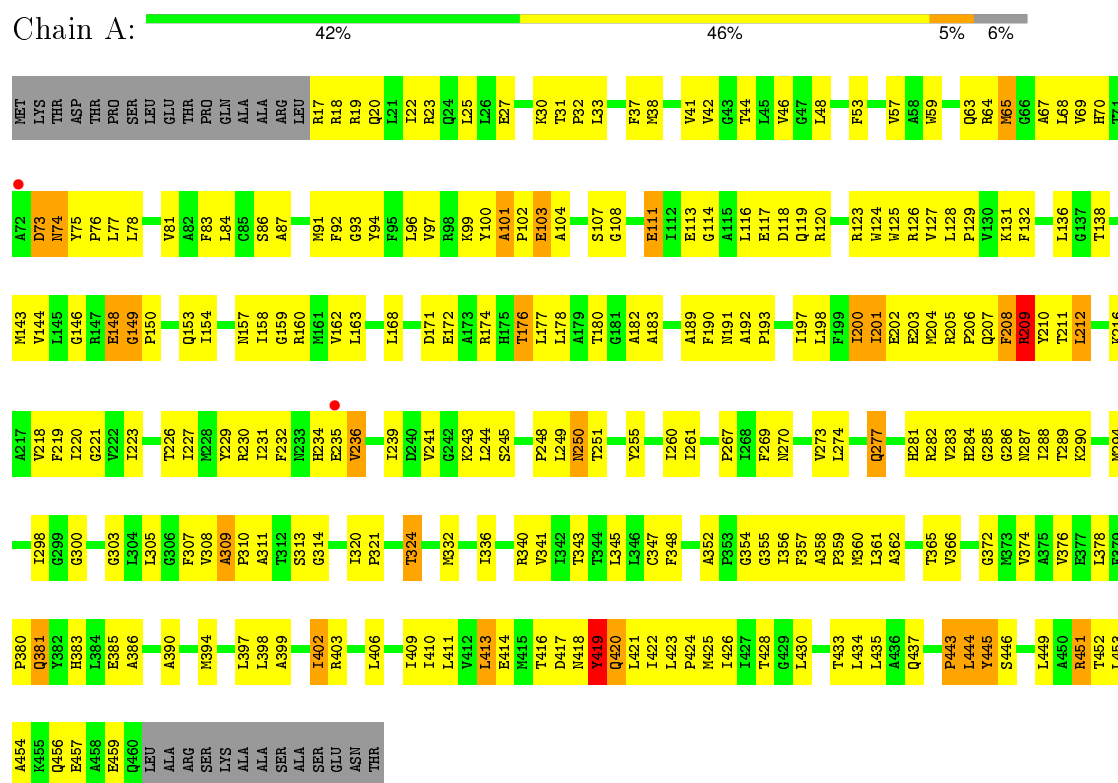
- Molecule 3 is a protein called Fab Fragment (Light Chain).

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			

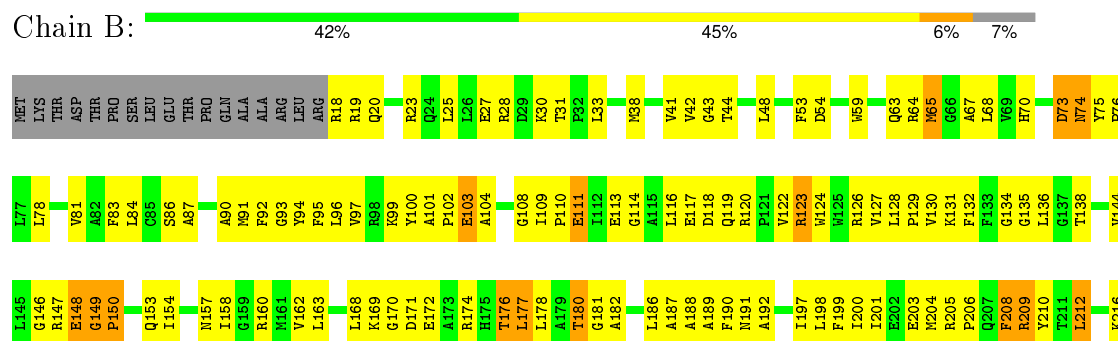
3 Residue-property plots

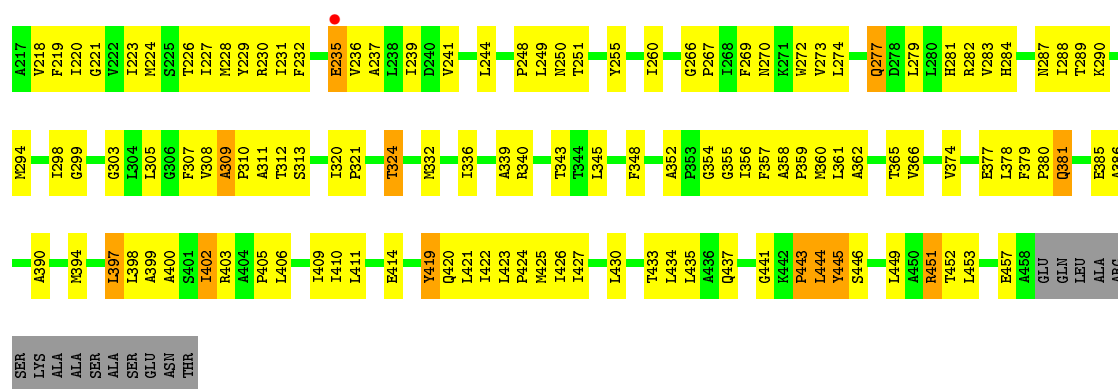
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

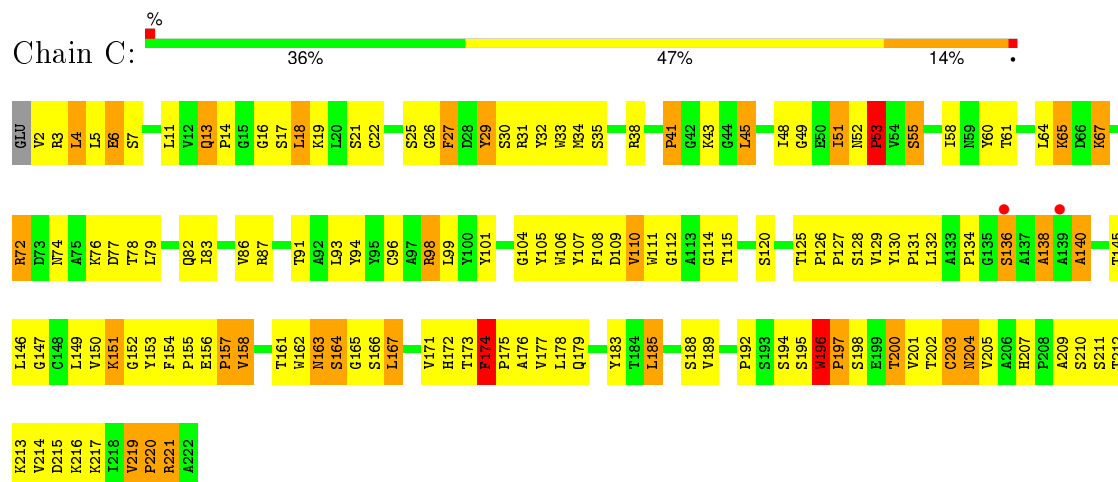


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

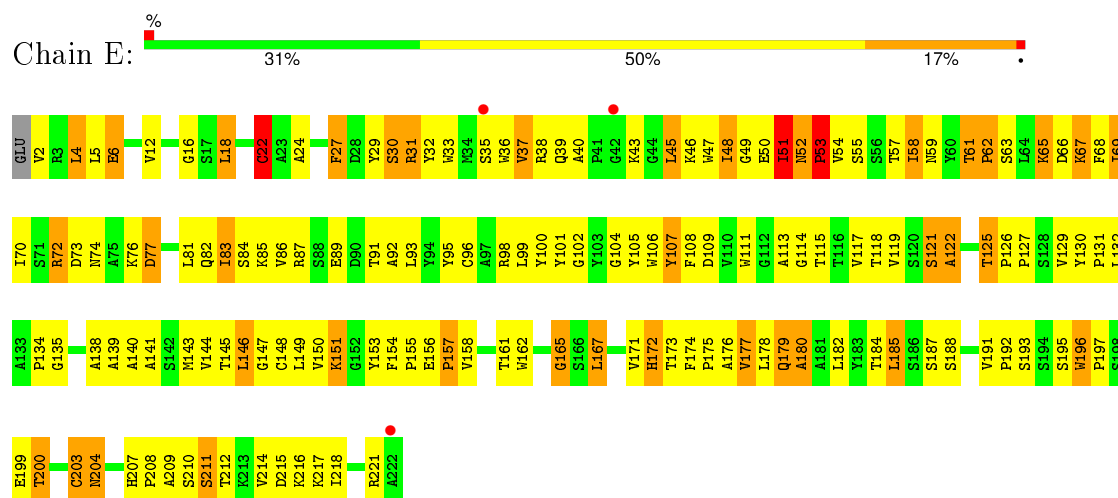




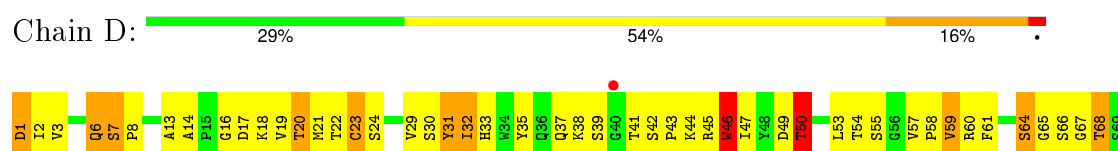
• Molecule 2: Fab Fragment (Heavy Chain)

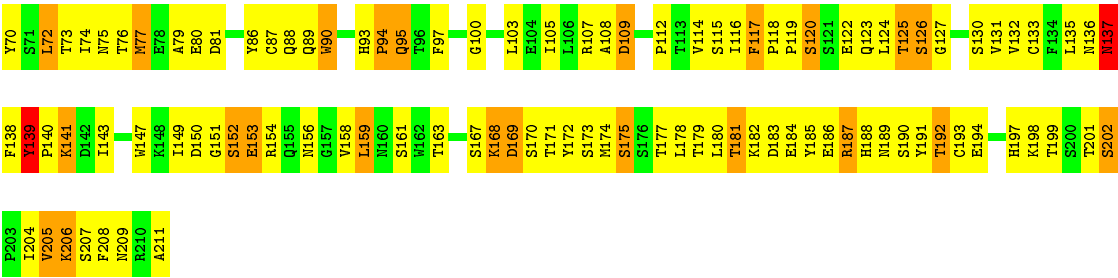


• Molecule 2: Fab Fragment (Heavy Chain)

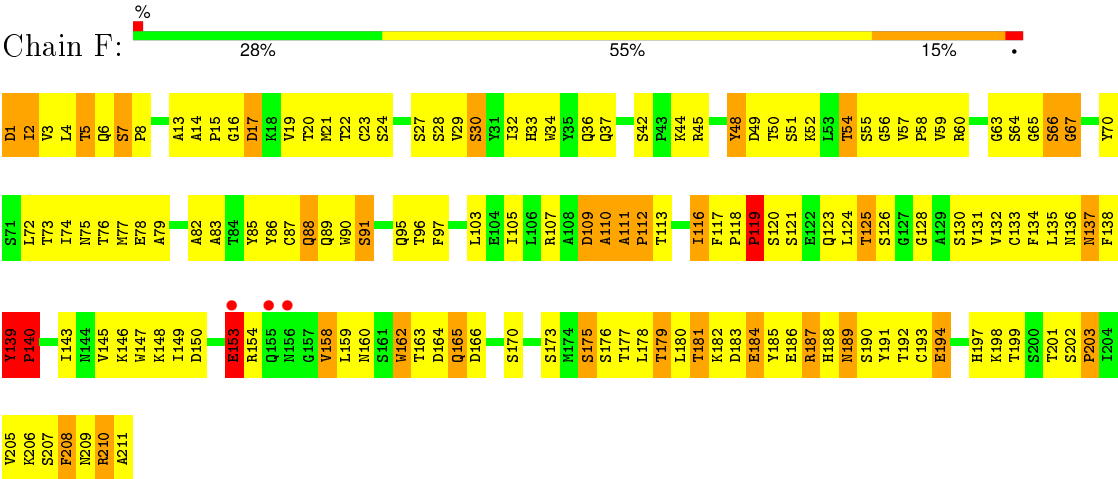


• Molecule 3: Fab Fragment (Light Chain)





● 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, α , β , γ	219.83Å 122.44Å 151.34Å 90.00° 128.16° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.98-3.20) 98.1 (19.98-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 3.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.268 , 0.314 0.261 , 0.292	Depositor DCC
R_{free} test set	2468 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 51930 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.43	0/3405	0.65	0/4621
1	B	0.48	0/3376	0.68	0/4583
2	C	0.56	0/1721	0.94	4/2355 (0.2%)
2	E	0.56	0/1721	0.94	4/2355 (0.2%)
3	D	0.44	0/1660	0.85	1/2257 (0.0%)
3	F	0.72	6/1660 (0.4%)	1.04	8/2257 (0.4%)
All	All	0.52	6/13543 (0.0%)	0.82	17/18428 (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
1	A	0	1
1	B	0	1
2	C	0	1
2	E	0	1
3	D	0	1
3	F	0	1
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	139	TYR	C-O	-8.93	1.06	1.23
3	F	140	PRO	CA-C	7.08	1.67	1.52
3	F	140	PRO	C-O	5.35	1.33	1.23
3	F	139	TYR	CD2-CE2	5.27	1.47	1.39
3	F	140	PRO	N-CA	5.16	1.56	1.47
3	F	139	TYR	CG-CD2	5.00	1.45	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	139	TYR	C-N-CA	-8.08	88.07	122.00
3	F	110	ALA	N-CA-C	7.11	130.20	111.00
3	F	140	PRO	CA-N-CD	-6.57	102.30	111.50
3	F	140	PRO	CA-C-O	6.33	135.38	120.20
2	E	22	CYS	CA-CB-SG	6.07	124.92	114.00
2	C	158	VAL	N-CA-C	-6.03	94.73	111.00
2	C	93	LEU	CA-CB-CG	5.52	127.99	115.30
2	C	196	TRP	N-CA-C	5.43	125.66	111.00
3	F	140	PRO	N-CA-C	5.42	126.19	112.10
2	C	61	THR	N-CA-C	-5.40	96.41	111.00
3	F	139	TYR	C-N-CD	5.28	139.48	128.40
3	D	139	TYR	C-N-CD	5.20	139.32	128.40
2	E	148	CYS	CA-CB-SG	5.18	123.33	114.00
3	F	140	PRO	CA-C-N	-5.17	105.82	117.20
2	E	31	ARG	CG-CD-NE	-5.17	100.95	111.80
2	E	102	GLY	N-CA-C	-5.11	100.32	113.10
3	F	139	TYR	N-CA-CB	5.10	119.77	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	TYR	Sidechain
1	B	419	TYR	Sidechain
2	C	29	TYR	Sidechain
3	D	139	TYR	Sidechain
2	E	101	TYR	Sidechain
3	F	139	TYR	Mainchain

5.2 Too-close contacts [i](#)

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	3333	0	3484	289	0
1	B	3304	0	3457	269	0
2	C	1672	0	1654	183	0
2	E	1672	0	1654	165	0
3	D	1621	0	1546	194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1621	0	1546	234	0
All	All	13223	0	13341	1220	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 46.

All (1220) 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)
2:E:207:HIS:ND1	2:E:210:SER:HB2	1.52	1.23
1:A:235:GLU:O	1:A:236:VAL:HG23	1.47	1.12
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.33	1.10
3:F:7:SER:HB2	3:F:22:THR:HB	1.34	1.08
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.35	1.07
3:F:192:THR:HA	3:F:207:SER:HB3	1.38	1.06
1:A:381:GLN:N	1:A:381:GLN:HE21	1.54	1.05
3:F:13:ALA:HB3	3:F:77:MET:HE1	1.39	1.03
2:C:51:ILE:HD11	2:C:55:SER:HB3	1.41	1.02
3:F:36:GLN:HG3	3:F:85:TYR:HE2	1.17	1.02
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.42	1.02
2:C:51:ILE:HD13	2:C:72:ARG:HD2	1.41	1.02
3:F:111:ALA:H	3:F:199:THR:HG21	1.25	1.01
1:B:381:GLN:N	1:B:381:GLN:HE21	1.57	1.01
3:F:139:TYR:O	3:F:140:PRO:C	1.86	1.01
1:B:287:ASN:ND2	1:B:290:LYS:H	1.58	1.00
3:D:31:TYR:HA	3:D:50:THR:OG1	1.61	1.00
1:A:381:GLN:NE2	1:A:381:GLN:H	1.59	0.99
1:B:381:GLN:H	1:B:381:GLN:NE2	1.61	0.99
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.44	0.99
2:C:177:VAL:HG21	3:D:159:LEU:HD13	1.43	0.97
1:A:287:ASN:ND2	1:A:290:LYS:H	1.60	0.97
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.44	0.96
1:A:216:LYS:HE2	1:B:433:THR:HG22	1.48	0.95
2:E:45:LEU:HD11	3:F:86:TYR:CD1	2.01	0.95
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.01	0.94
3:D:22:THR:HG22	3:D:23:CYS:H	1.30	0.94
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.31	0.94
1:A:457:GLU:HG3	1:B:18:ARG:HH11	1.32	0.94
3:F:190:SER:HA	3:F:209:ASN:OD1	1.69	0.93
3:F:65:GLY:HA3	3:F:70:TYR:CD2	2.04	0.92
2:C:2:VAL:HG23	2:C:27:PHE:CD1	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.01	0.91
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.53	0.91
1:B:176:THR:O	1:B:180:THR:HG23	1.71	0.91
3:F:139:TYR:O	3:F:140:PRO:O	1.88	0.91
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.53	0.90
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.50	0.90
3:F:36:GLN:HG3	3:F:85:TYR:CE2	2.06	0.90
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.54	0.90
3:F:14:ALA:O	3:F:17:ASP:HB2	1.70	0.89
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.51	0.89
1:A:212:LEU:H	1:A:212:LEU:HD12	1.38	0.89
1:B:320:ILE:HG21	1:B:394:MET:HE1	1.54	0.89
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.09	0.88
3:F:20:THR:HG23	3:F:73:THR:OG1	1.74	0.88
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.55	0.87
2:E:207:HIS:ND1	2:E:210:SER:CB	2.38	0.87
1:B:212:LEU:HD12	1:B:212:LEU:H	1.40	0.86
3:D:95:GLN:H	3:D:95:GLN:CD	1.72	0.86
2:C:35:SER:HB2	2:C:49:GLY:O	1.76	0.86
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.58	0.86
2:C:178:LEU:HD12	2:C:179:GLN:H	1.41	0.85
3:F:111:ALA:N	3:F:199:THR:HG21	1.90	0.85
1:A:433:THR:HG22	1:B:216:LYS:HE2	1.60	0.84
1:A:250:ASN:HD22	2:C:105:TYR:HE1	1.23	0.83
3:D:150:ASP:HA	3:D:190:SER:HB3	1.59	0.83
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.14	0.83
2:C:132:LEU:HB2	2:C:147:GLY:O	1.79	0.83
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.59	0.83
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.60	0.83
3:F:153:GLU:HG3	3:F:154:ARG:N	1.92	0.82
2:C:129:VAL:HG21	2:C:214:VAL:HG21	1.59	0.82
3:D:95:GLN:N	3:D:95:GLN:OE1	2.12	0.82
3:D:112:PRO:HG2	3:D:204:ILE:HD12	1.61	0.81
2:C:147:GLY:HA2	2:C:162:TRP:HH2	1.44	0.81
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.62	0.81
3:F:192:THR:CA	3:F:207:SER:HB3	2.10	0.81
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.61	0.81
2:C:147:GLY:HA2	2:C:162:TRP:CH2	2.15	0.80
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.10	0.80
2:C:98:ARG:HD2	2:C:110:VAL:HG23	1.61	0.80
2:E:91:THR:OG1	2:E:119:VAL:HG23	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:HB1	1:A:414:GLU:OE2	1.80	0.80
3:F:7:SER:HB3	3:F:8:PRO:CD	2.12	0.79
2:E:16:GLY:H	2:E:86:VAL:HG22	1.46	0.79
1:A:200:ILE:HA	1:A:204:MET:HB2	1.64	0.79
3:D:13:ALA:HB3	3:D:77:MET:HE3	1.62	0.79
2:E:125:THR:HG22	2:E:153:TYR:HA	1.64	0.79
2:E:18:LEU:H	2:E:18:LEU:HD23	1.48	0.79
3:D:14:ALA:O	3:D:17:ASP:HB2	1.82	0.78
1:B:227:ILE:O	1:B:231:ILE:HG12	1.84	0.78
1:A:171:ASP:HB2	1:A:212:LEU:HD22	1.65	0.78
1:A:457:GLU:HG3	1:B:18:ARG:NH1	1.98	0.78
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.14	0.78
3:D:54:THR:O	3:D:57:VAL:HG23	1.84	0.78
3:F:210:ARG:HB3	3:F:210:ARG:NH1	1.98	0.77
3:D:13:ALA:HB3	3:D:77:MET:CE	2.13	0.77
1:B:200:ILE:HA	1:B:204:MET:HB2	1.66	0.77
1:B:409:ILE:HD13	1:B:426:ILE:HG12	1.66	0.77
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.66	0.77
1:A:320:ILE:HD13	1:A:394:MET:CE	2.15	0.77
3:F:7:SER:CB	3:F:8:PRO:HD3	2.14	0.77
1:B:171:ASP:HB2	1:B:212:LEU:HD22	1.67	0.77
1:B:127:VAL:HB	1:B:157:ASN:ND2	1.99	0.77
1:B:200:ILE:HG22	1:B:201:ILE:N	2.00	0.77
1:A:208:PHE:O	1:A:209:ARG:HB3	1.85	0.76
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.20	0.76
3:D:158:VAL:O	3:D:159:LEU:HD23	1.85	0.76
2:C:196:TRP:O	2:C:197:PRO:C	2.20	0.76
1:A:398:LEU:O	1:A:402:ILE:HG23	1.85	0.76
1:A:18:ARG:NH1	1:B:457:GLU:HB3	2.00	0.76
1:B:208:PHE:O	1:B:209:ARG:HB3	1.85	0.76
2:C:174:PHE:H	2:C:174:PHE:HD2	1.30	0.76
2:E:73:ASP:OD2	2:E:76:LYS:HD2	1.86	0.76
1:B:59:TRP:O	1:B:63:GLN:HG2	1.86	0.76
3:D:7:SER:HB2	3:D:22:THR:HB	1.67	0.76
2:C:30:SER:C	2:C:32:TYR:H	1.85	0.76
1:A:86:SER:OG	1:A:303:GLY:HA3	1.85	0.76
3:F:124:LEU:HD23	3:F:128:GLY:O	1.87	0.75
3:F:22:THR:HG22	3:F:23:CYS:N	1.99	0.75
1:B:131:LYS:HE3	1:B:150:PRO:HA	1.68	0.75
2:E:204:ASN:HB3	2:E:215:ASP:OD1	1.85	0.75
3:D:125:THR:HG22	3:D:125:THR:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:ILE:HD11	3:F:27:SER:HB2	1.68	0.74
2:C:2:VAL:HG23	2:C:27:PHE:HD1	1.48	0.74
3:F:48:TYR:CE2	3:F:52:LYS:HB2	2.23	0.74
1:B:423:LEU:HB3	1:B:424:PRO:HD3	1.70	0.74
3:F:188:HIS:O	3:F:210:ARG:HD3	1.87	0.74
2:E:107:TYR:HE2	3:F:48:TYR:CD1	2.06	0.74
3:D:90:TRP:CE2	3:D:95:GLN:NE2	2.56	0.74
3:F:19:VAL:HG12	3:F:74:ILE:HB	1.68	0.74
3:D:6:GLN:HG3	3:D:100:GLY:H	1.52	0.74
2:C:172:HIS:HB2	2:C:188:SER:HB3	1.70	0.74
2:E:61:THR:O	2:E:63:SER:N	2.21	0.74
2:C:51:ILE:HD11	2:C:55:SER:CB	2.18	0.73
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.68	0.73
1:A:38:MET:HA	1:A:41:VAL:HG12	1.70	0.73
2:E:100:TYR:HB3	2:E:107:TYR:HE1	1.54	0.73
2:C:129:VAL:HG21	2:C:214:VAL:CG2	2.18	0.73
1:A:234:HIS:CE1	3:F:52:LYS:NZ	2.57	0.73
1:A:248:PRO:O	1:A:251:THR:HB	1.89	0.73
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.52	0.73
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.51	0.73
3:F:187:ARG:HG2	3:F:188:HIS:CD2	2.24	0.72
1:B:320:ILE:HD13	1:B:394:MET:CE	2.20	0.72
3:D:60:ARG:HG2	3:D:74:ILE:HG22	1.71	0.72
2:C:72:ARG:NH1	2:C:74:ASN:OD1	2.22	0.72
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.18	0.72
3:D:136:ASN:HB3	3:D:137:ASN:ND2	2.05	0.72
3:F:95:GLN:OE1	3:F:95:GLN:N	2.23	0.72
1:A:419:TYR:CZ	1:B:414:GLU:HG2	2.24	0.72
3:F:116:ILE:HD12	3:F:193:CYS:HB2	1.70	0.72
3:F:210:ARG:CG	3:F:210:ARG:HH11	2.02	0.71
1:B:154:ILE:O	1:B:158:ILE:HG12	1.89	0.71
3:F:7:SER:CB	3:F:22:THR:HB	2.16	0.71
3:F:149:ILE:HD12	3:F:154:ARG:HH11	1.55	0.71
2:C:52:ASN:HB2	2:C:53:PRO:HD2	1.72	0.71
1:A:294:MET:O	1:A:298:ILE:HG13	1.90	0.71
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.59	0.70
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.56	0.70
1:A:17:ARG:HG3	1:A:18:ARG:N	2.05	0.70
2:E:36:TRP:O	2:E:37:VAL:HG23	1.91	0.70
2:C:177:VAL:HG21	3:D:159:LEU:CD1	2.21	0.70
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:ASP:HA	3:D:45:ARG:HE	1.56	0.70
1:B:212:LEU:HD12	1:B:212:LEU:N	2.06	0.70
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.56	0.70
2:E:30:SER:O	2:E:31:ARG:HB2	1.91	0.70
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.74	0.70
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.73	0.70
1:A:332:MET:O	1:A:336:ILE:HG13	1.91	0.70
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.22	0.69
3:F:22:THR:CG2	3:F:23:CYS:N	2.55	0.69
3:D:201:THR:HG23	3:D:202:SER:H	1.58	0.69
1:A:451:ARG:HB3	1:A:451:ARG:HH11	1.56	0.69
3:F:82:ALA:HB2	3:F:105:ILE:CD1	2.22	0.69
3:F:72:LEU:HD23	3:F:72:LEU:C	2.13	0.69
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.58	0.69
1:A:20:GLN:O	1:A:23:ARG:HB3	1.93	0.69
2:C:196:TRP:O	2:C:198:SER:N	2.26	0.69
2:C:6:GLU:O	2:C:115:THR:HG23	1.93	0.69
1:A:409:ILE:HD13	1:A:426:ILE:HG12	1.75	0.69
3:F:150:ASP:HA	3:F:190:SER:HB3	1.75	0.68
3:F:134:PHE:O	3:F:135:LEU:HD23	1.93	0.68
1:A:200:ILE:HG22	1:A:201:ILE:N	2.07	0.68
2:E:39:GLN:O	2:E:92:ALA:HB1	1.93	0.68
1:A:414:GLU:HG2	1:B:419:TYR:CZ	2.28	0.68
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.58	0.68
3:D:123:GLN:HE22	3:D:130:SER:HB2	1.57	0.68
1:B:108:GLY:HA3	1:B:153:GLN:NE2	2.08	0.68
1:B:374:VAL:O	1:B:378:LEU:HG	1.94	0.68
3:D:125:THR:O	3:D:125:THR:CG2	2.42	0.68
1:A:287:ASN:HD22	1:A:290:LYS:H	1.41	0.68
3:F:197:HIS:CE1	3:F:199:THR:HG23	2.29	0.68
2:E:146:LEU:HD23	2:E:146:LEU:N	2.08	0.68
2:C:51:ILE:CD1	2:C:55:SER:HB3	2.21	0.68
3:D:94:PRO:HA	3:D:95:GLN:OE1	1.92	0.68
3:D:6:GLN:OE1	3:D:87:CYS:N	2.23	0.68
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.28	0.68
3:F:88:GLN:HB2	3:F:97:PHE:HD1	1.59	0.67
3:F:72:LEU:HD23	3:F:73:THR:N	2.08	0.67
1:B:443:PRO:O	1:B:446:SER:N	2.28	0.67
3:F:7:SER:CB	3:F:8:PRO:CD	2.70	0.67
2:C:29:TYR:OH	2:C:34:MET:HG3	1.93	0.67
3:F:32:ILE:CD1	3:F:89:GLN:HB3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.28	0.67
1:B:287:ASN:HD22	1:B:290:LYS:H	1.38	0.67
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.77	0.67
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.29	0.67
1:B:74:ASN:HD22	1:B:75:TYR:N	1.93	0.67
1:B:127:VAL:HB	1:B:157:ASN:HD21	1.58	0.67
3:F:2:ILE:CD1	3:F:27:SER:HB2	2.24	0.67
1:A:320:ILE:HG23	1:A:365:THR:HG21	1.77	0.67
3:F:37:GLN:O	3:F:83:ALA:HB1	1.94	0.67
2:E:196:TRP:HB3	2:E:197:PRO:HD3	1.77	0.67
2:C:51:ILE:CD1	2:C:72:ARG:HD2	2.24	0.67
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.76	0.66
1:B:38:MET:HA	1:B:41:VAL:HG12	1.78	0.66
1:A:235:GLU:O	1:A:236:VAL:CG2	2.34	0.66
3:F:7:SER:O	3:F:8:PRO:C	2.32	0.66
1:A:176:THR:HG22	1:A:177:LEU:HD23	1.77	0.66
2:C:45:LEU:H	2:C:45:LEU:HD12	1.61	0.66
2:C:30:SER:O	2:C:32:TYR:N	2.25	0.66
3:F:13:ALA:HB3	3:F:77:MET:CE	2.22	0.66
1:A:255:TYR:HB3	1:A:428:THR:OG1	1.95	0.66
1:A:92:PHE:O	1:A:96:LEU:HD23	1.96	0.66
3:F:210:ARG:HG2	3:F:210:ARG:HH11	1.59	0.66
2:C:204:ASN:HB3	2:C:215:ASP:OD1	1.96	0.66
1:B:294:MET:O	1:B:298:ILE:HG13	1.96	0.66
1:A:150:PRO:O	1:A:154:ILE:HG13	1.96	0.66
3:D:22:THR:HG22	3:D:23:CYS:N	2.06	0.66
3:F:148:LYS:HB2	3:F:192:THR:OG1	1.95	0.65
2:C:105:TYR:CD2	3:D:31:TYR:HD1	2.14	0.65
3:F:192:THR:HA	3:F:207:SER:CB	2.23	0.65
3:D:50:THR:HG23	3:D:70:TYR:CD2	2.31	0.65
2:E:108:PHE:CE1	3:F:88:GLN:NE2	2.64	0.65
2:C:26:GLY:O	2:C:27:PHE:HB3	1.96	0.65
2:C:192:PRO:O	2:C:195:SER:HB3	1.95	0.65
2:E:145:THR:C	2:E:146:LEU:HD23	2.17	0.65
3:F:187:ARG:HG3	3:F:187:ARG:O	1.97	0.65
1:A:87:ALA:O	1:A:91:MET:HG3	1.97	0.65
2:E:108:PHE:CD1	3:F:88:GLN:NE2	2.64	0.65
1:A:234:HIS:CE1	3:F:52:LYS:HZ1	2.14	0.65
3:F:194:GLU:CG	3:F:205:VAL:HG12	2.25	0.65
1:B:287:ASN:ND2	1:B:290:LYS:N	2.39	0.65
2:E:45:LEU:HD11	3:F:86:TYR:CE1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HE3	1:A:150:PRO:HA	1.79	0.65
2:E:132:LEU:HD13	3:F:132:VAL:HG21	1.79	0.65
1:B:421:LEU:O	1:B:424:PRO:HD2	1.97	0.64
1:A:154:ILE:O	1:A:158:ILE:HG12	1.97	0.64
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.32	0.64
1:A:449:LEU:O	1:A:453:LEU:HB2	1.98	0.64
3:F:158:VAL:HG23	3:F:178:LEU:HD13	1.79	0.64
1:B:332:MET:O	1:B:336:ILE:HG13	1.97	0.64
1:A:176:THR:O	1:A:180:THR:HG23	1.98	0.64
1:A:320:ILE:HD13	1:A:394:MET:HE1	1.80	0.64
3:D:117:PHE:N	3:D:117:PHE:CD1	2.64	0.64
3:D:180:LEU:HD12	3:D:185:TYR:HB2	1.78	0.64
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.33	0.64
3:D:31:TYR:HA	3:D:50:THR:HG1	1.60	0.64
2:C:32:TYR:CE2	2:C:98:ARG:NE	2.66	0.64
3:F:82:ALA:HB2	3:F:105:ILE:HD11	1.80	0.64
2:E:6:GLU:HA	2:E:22:CYS:HA	1.80	0.64
3:D:47:ILE:HG13	3:D:53:LEU:HD23	1.80	0.63
1:A:443:PRO:O	1:A:446:SER:N	2.30	0.63
1:B:92:PHE:O	1:B:96:LEU:HD23	1.98	0.63
3:D:95:GLN:N	3:D:95:GLN:CD	2.48	0.63
3:D:182:LYS:HG2	3:D:186:GLU:OE1	1.98	0.63
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.12	0.63
1:B:20:GLN:O	1:B:23:ARG:HB3	1.98	0.63
3:D:50:THR:HG23	3:D:70:TYR:HD2	1.64	0.63
3:F:45:ARG:HH12	3:F:54:THR:HG23	1.63	0.63
1:A:399:ALA:O	1:A:403:ARG:HA	1.99	0.63
3:F:77:MET:SD	3:F:103:LEU:HD21	2.38	0.63
1:A:38:MET:HG3	1:A:168:LEU:CD1	2.28	0.63
2:E:130:TYR:HB3	3:F:120:SER:OG	1.98	0.63
1:B:451:ARG:HB3	1:B:451:ARG:HH11	1.64	0.63
1:A:423:LEU:HB3	1:A:424:PRO:CD	2.21	0.63
1:B:74:ASN:O	1:B:78:LEU:HB2	1.99	0.63
3:F:178:LEU:HD12	3:F:179:THR:N	2.14	0.63
1:B:86:SER:OG	1:B:303:GLY:HA3	1.99	0.63
3:F:182:LYS:O	3:F:186:GLU:HG3	1.99	0.63
1:A:226:THR:O	1:A:230:ARG:HG2	1.99	0.63
2:C:2:VAL:HG13	2:C:2:VAL:O	1.99	0.63
2:E:196:TRP:O	2:E:197:PRO:C	2.36	0.63
1:A:172:GLU:O	1:A:176:THR:HB	1.99	0.62
2:C:32:TYR:HD2	2:C:98:ARG:HG2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:146:LYS:HD3	3:F:148:LYS:HE3	1.80	0.62
3:F:210:ARG:HB3	3:F:210:ARG:HH11	1.63	0.62
1:A:212:LEU:N	1:A:212:LEU:HD12	2.10	0.62
1:B:320:ILE:HG23	1:B:365:THR:HG21	1.81	0.62
3:D:117:PHE:N	3:D:117:PHE:HD1	1.97	0.62
2:C:192:PRO:HB2	2:C:195:SER:HB2	1.80	0.62
1:A:59:TRP:O	1:A:63:GLN:HG2	1.98	0.62
2:C:22:CYS:O	2:C:78:THR:HG23	2.00	0.62
2:C:174:PHE:N	2:C:174:PHE:CD2	2.60	0.62
2:E:108:PHE:HE1	3:F:88:GLN:HE21	1.44	0.62
1:B:176:THR:HG22	1:B:177:LEU:HD23	1.81	0.62
3:F:153:GLU:HG3	3:F:154:ARG:H	1.64	0.62
3:F:133:CYS:HB2	3:F:147:TRP:CH2	2.34	0.62
2:E:33:TRP:CH2	2:E:52:ASN:HB3	2.35	0.62
3:F:210:ARG:CB	3:F:210:ARG:HH11	2.12	0.62
2:C:32:TYR:CD2	2:C:98:ARG:HG2	2.35	0.62
2:E:33:TRP:O	2:E:99:LEU:HB2	2.01	0.61
3:F:187:ARG:CG	3:F:187:ARG:O	2.47	0.61
2:C:178:LEU:HD12	2:C:179:GLN:N	2.12	0.61
3:D:201:THR:HG23	3:D:202:SER:N	2.14	0.61
1:A:374:VAL:O	1:A:378:LEU:HG	2.00	0.61
2:E:162:TRP:CZ3	2:E:203:CYS:CB	2.81	0.61
1:A:148:GLU:OE1	1:A:355:GLY:HA3	2.00	0.61
3:F:125:THR:O	3:F:125:THR:HG22	1.99	0.61
2:C:172:HIS:HD2	3:D:136:ASN:ND2	1.97	0.61
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.35	0.61
3:F:107:ARG:HD3	3:F:170:SER:O	2.00	0.61
3:D:30:SER:HA	3:D:70:TYR:OH	2.01	0.61
2:E:18:LEU:N	2:E:18:LEU:HD23	2.13	0.61
3:D:168:LYS:O	3:D:170:SER:N	2.33	0.61
3:F:34:TRP:CZ2	3:F:72:LEU:HB2	2.36	0.61
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.35	0.61
3:D:7:SER:CB	3:D:8:PRO:HD3	2.31	0.61
1:A:239:ILE:HD13	1:A:394:MET:HE1	1.83	0.61
3:D:136:ASN:HB3	3:D:137:ASN:HD22	1.66	0.61
2:C:7:SER:HA	2:C:115:THR:HG21	1.82	0.61
1:A:274:LEU:HD23	1:A:277:GLN:HE22	1.65	0.61
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.36	0.61
1:B:87:ALA:O	1:B:91:MET:HG3	2.01	0.61
3:F:191:TYR:HB2	3:F:208:PHE:CE2	2.34	0.61
1:A:108:GLY:HA3	1:A:153:GLN:NE2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:TRP:HE3	2:E:95:TYR:O	1.82	0.61
2:C:105:TYR:CE2	3:D:31:TYR:HD1	2.19	0.60
2:E:200:THR:OG1	2:E:217:LYS:HE3	2.01	0.60
3:D:143:ILE:HG23	3:D:174:MET:CE	2.30	0.60
1:A:113:GLU:OE2	1:A:203:GLU:HG3	2.00	0.60
1:A:31:THR:H	1:B:437:GLN:HE22	1.47	0.60
3:F:139:TYR:CG	3:F:140:PRO:N	2.70	0.60
1:B:163:LEU:CD2	1:B:174:ARG:HA	2.31	0.60
1:A:269:PHE:O	1:A:273:VAL:HG12	2.00	0.60
3:D:17:ASP:O	3:D:76:THR:HA	2.01	0.60
1:A:74:ASN:O	1:A:78:LEU:HB2	2.00	0.60
3:D:139:TYR:CD1	3:D:140:PRO:HD3	2.37	0.60
1:A:409:ILE:HD11	1:A:426:ILE:HA	1.84	0.60
2:C:30:SER:C	2:C:32:TYR:N	2.55	0.60
1:A:171:ASP:CB	1:A:212:LEU:HD22	2.31	0.60
3:D:192:THR:HA	3:D:207:SER:HB3	1.84	0.60
3:D:137:ASN:HA	3:D:172:TYR:O	2.02	0.60
2:C:200:THR:HG22	2:C:200:THR:O	2.00	0.60
2:E:107:TYR:HE2	3:F:48:TYR:HD1	1.47	0.60
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.84	0.60
1:B:273:VAL:HA	1:B:345:LEU:HD22	1.83	0.60
2:E:179:GLN:O	2:E:180:ALA:HB3	2.02	0.60
2:C:156:GLU:OE2	2:C:176:ALA:HB3	2.02	0.60
1:B:131:LYS:HE2	1:B:153:GLN:NE2	2.15	0.59
1:A:220:ILE:HG13	1:B:430:LEU:HD21	1.84	0.59
2:E:69:ILE:O	2:E:69:ILE:HG22	2.02	0.59
2:E:69:ILE:HB	2:E:82:GLN:HB2	1.85	0.59
1:A:99:LYS:HG2	1:A:100:TYR:CE1	2.37	0.59
2:E:132:LEU:CD1	3:F:132:VAL:HG21	2.32	0.59
1:B:248:PRO:O	1:B:251:THR:HB	2.03	0.59
1:A:250:ASN:ND2	2:C:105:TYR:CE1	2.62	0.59
1:B:117:GLU:OE1	1:B:209:ARG:NH1	2.34	0.59
3:F:178:LEU:HD12	3:F:179:THR:H	1.67	0.59
3:F:197:HIS:ND1	3:F:198:LYS:N	2.49	0.59
1:A:249:LEU:C	1:A:251:THR:H	2.04	0.59
2:E:144:VAL:O	2:E:144:VAL:HG13	2.01	0.59
1:A:108:GLY:HA3	1:A:153:GLN:HE21	1.68	0.59
1:A:383:HIS:CE1	3:D:90:TRP:CZ2	2.91	0.59
3:D:46:TRP:HA	3:D:46:TRP:CE3	2.37	0.59
1:A:357:PHE:CE1	1:A:398:LEU:HD22	2.37	0.59
3:F:116:ILE:CD1	3:F:193:CYS:HB2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:PRO:HB2	2:E:195:SER:HB2	1.82	0.59
1:A:223:ILE:CD1	1:B:426:ILE:HG22	2.22	0.59
3:D:114:VAL:O	3:D:206:LYS:HD2	2.03	0.59
3:D:21:MET:SD	3:D:72:LEU:HD22	2.43	0.59
3:D:89:GLN:OE1	3:D:90:TRP:N	2.36	0.59
3:D:190:SER:HA	3:D:209:ASN:OD1	2.03	0.59
2:C:45:LEU:HD11	3:D:86:TYR:CD1	2.37	0.59
1:A:220:ILE:CG1	1:B:430:LEU:HD21	2.32	0.59
2:C:38:ARG:HD3	2:C:48:ILE:HD11	1.84	0.59
3:F:65:GLY:HA3	3:F:70:TYR:HD2	1.66	0.59
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.35	0.59
3:D:79:ALA:HB1	3:D:105:ILE:CD1	2.33	0.58
1:A:212:LEU:H	1:A:212:LEU:CD1	2.14	0.58
3:D:141:LYS:HB3	3:D:172:TYR:CD1	2.38	0.58
3:F:45:ARG:NH1	3:F:54:THR:HG23	2.18	0.58
1:A:33:LEU:O	1:A:33:LEU:HD23	2.02	0.58
3:F:188:HIS:O	3:F:210:ARG:CD	2.50	0.58
1:B:241:VAL:HG11	1:B:324:THR:HG21	1.85	0.58
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.18	0.58
1:A:414:GLU:HG2	1:B:419:TYR:OH	2.02	0.58
2:E:131:PRO:HD3	2:E:216:LYS:HG2	1.83	0.58
3:F:205:VAL:O	3:F:206:LYS:HG2	2.03	0.58
2:C:146:LEU:HB2	2:C:189:VAL:CG1	2.33	0.58
3:F:64:SER:OG	3:F:65:GLY:N	2.37	0.58
1:B:27:GLU:O	1:B:30:LYS:HG3	2.02	0.58
1:A:160:ARG:O	1:A:163:LEU:HB3	2.04	0.58
1:A:202:GLU:O	1:A:202:GLU:HG2	2.02	0.58
3:F:89:GLN:HE21	3:F:96:THR:H	1.50	0.58
2:C:150:VAL:CG2	2:C:205:VAL:HG21	2.33	0.58
3:D:94:PRO:CA	3:D:95:GLN:OE1	2.51	0.58
3:F:21:MET:SD	3:F:85:TYR:HD1	2.26	0.58
3:F:89:GLN:NE2	3:F:95:GLN:HA	2.19	0.57
2:E:40:ALA:HA	2:E:92:ALA:HB2	1.86	0.57
3:D:141:LYS:HB3	3:D:172:TYR:CE1	2.39	0.57
2:C:177:VAL:CG2	3:D:159:LEU:HD13	2.26	0.57
3:F:189:ASN:ND2	3:F:210:ARG:HB2	2.18	0.57
1:B:449:LEU:O	1:B:453:LEU:HB2	2.03	0.57
1:A:372:GLY:O	1:A:376:VAL:HG23	2.04	0.57
1:A:287:ASN:ND2	1:A:290:LYS:N	2.42	0.57
1:B:172:GLU:O	1:B:176:THR:HB	2.05	0.57
2:C:185:LEU:HD12	2:C:185:LEU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG11	1:B:444:LEU:HD21	1.86	0.57
2:C:17:SER:O	2:C:18:LEU:HB3	2.04	0.57
2:C:173:THR:O	2:C:173:THR:HG22	2.03	0.57
3:F:73:THR:HG22	3:F:74:ILE:N	2.17	0.57
1:A:74:ASN:HD22	1:A:75:TYR:N	2.02	0.57
1:B:208:PHE:N	1:B:208:PHE:CD1	2.70	0.57
1:A:198:LEU:HD11	1:B:198:LEU:HD21	1.85	0.57
3:F:73:THR:CG2	3:F:74:ILE:N	2.66	0.57
1:B:160:ARG:O	1:B:163:LEU:N	2.35	0.57
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.86	0.57
2:E:158:VAL:HG21	2:E:185:LEU:HD11	1.86	0.57
1:A:53:PHE:O	1:A:57:VAL:HG23	2.04	0.57
1:B:380:PRO:HD2	1:B:381:GLN:NE2	2.19	0.57
2:C:132:LEU:HB3	3:D:117:PHE:CD2	2.38	0.57
3:F:32:ILE:HG22	3:F:33:HIS:N	2.20	0.57
3:D:81:ASP:O	3:D:103:LEU:HD23	2.05	0.57
1:B:38:MET:HG3	1:B:168:LEU:CD1	2.30	0.57
2:E:171:VAL:C	2:E:172:HIS:HD1	2.07	0.57
1:B:398:LEU:O	1:B:402:ILE:HG23	2.04	0.57
1:B:191:ASN:HB2	1:B:229:TYR:CE2	2.40	0.57
1:B:163:LEU:HD21	1:B:174:ARG:HA	1.86	0.57
2:C:162:TRP:CE2	2:C:189:VAL:HB	2.40	0.57
3:D:114:VAL:HG22	3:D:135:LEU:CD2	2.34	0.57
2:E:107:TYR:CE2	3:F:48:TYR:HD1	2.22	0.56
1:B:65:MET:C	1:B:67:ALA:H	2.08	0.56
3:F:22:THR:CG2	3:F:23:CYS:H	2.17	0.56
2:E:32:TYR:O	2:E:72:ARG:NH2	2.38	0.56
1:A:250:ASN:ND2	2:C:105:TYR:HE1	2.00	0.56
3:D:7:SER:CB	3:D:22:THR:HB	2.34	0.56
1:A:192:ALA:HB1	1:A:414:GLU:CD	2.24	0.56
1:B:150:PRO:O	1:B:154:ILE:HG13	2.05	0.56
3:F:15:PRO:HD3	3:F:105:ILE:HG23	1.88	0.56
2:C:16:GLY:O	2:C:86:VAL:HG13	2.04	0.56
3:F:192:THR:HG22	3:F:207:SER:CB	2.35	0.56
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.19	0.56
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.34	0.56
1:B:160:ARG:HH12	1:B:174:ARG:HD2	1.69	0.56
2:C:150:VAL:HB	2:C:185:LEU:CD1	2.36	0.56
2:C:213:LYS:O	2:C:214:VAL:HG13	2.04	0.56
2:E:68:PHE:CD2	2:E:83:ILE:HG23	2.41	0.56
1:B:212:LEU:CD1	1:B:212:LEU:H	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:ARG:HD2	2:C:110:VAL:CG2	2.33	0.56
1:A:410:ILE:O	1:A:414:GLU:HB2	2.06	0.56
3:D:138:PHE:CE1	3:D:172:TYR:HB2	2.41	0.56
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.04	0.56
1:A:311:ALA:HB1	1:A:336:ILE:HD13	1.88	0.56
3:F:159:LEU:O	3:F:177:THR:N	2.31	0.56
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.88	0.56
3:D:93:HIS:CD2	3:D:94:PRO:HB3	2.40	0.56
3:F:110:ALA:HB3	3:F:139:TYR:N	2.20	0.56
1:A:17:ARG:HG3	1:A:18:ARG:H	1.69	0.56
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.88	0.56
2:E:107:TYR:HB3	3:F:33:HIS:NE2	2.18	0.56
1:A:198:LEU:HD21	1:B:198:LEU:HD11	1.88	0.56
2:C:2:VAL:HA	2:C:25:SER:O	2.06	0.56
1:A:116:LEU:CD2	1:A:178:LEU:HD23	2.33	0.56
1:A:146:GLY:HA3	1:A:148:GLU:OE2	2.06	0.56
2:E:200:THR:O	2:E:200:THR:HG22	2.05	0.56
2:E:221:ARG:HD2	3:F:118:PRO:HG2	1.87	0.55
1:A:119:GLN:HB3	1:A:453:LEU:HD11	1.88	0.55
3:F:149:ILE:HD12	3:F:154:ARG:NH1	2.20	0.55
2:E:195:SER:O	2:E:199:GLU:HG3	2.06	0.55
1:A:144:VAL:HG21	1:A:343:THR:HB	1.88	0.55
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.87	0.55
1:B:274:LEU:O	1:B:277:GLN:HB2	2.06	0.55
1:B:113:GLU:OE2	1:B:203:GLU:HG3	2.07	0.55
2:E:207:HIS:CE1	2:E:210:SER:HB2	2.37	0.55
3:F:118:PRO:O	3:F:119:PRO:C	2.44	0.55
1:B:284:HIS:HA	1:B:290:LYS:HB3	1.89	0.55
2:E:32:TYR:CE2	2:E:98:ARG:HD3	2.41	0.55
2:E:132:LEU:HB2	2:E:147:GLY:O	2.07	0.55
1:B:218:VAL:O	1:B:221:GLY:N	2.39	0.55
1:B:226:THR:O	1:B:230:ARG:HG2	2.07	0.55
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.20	0.55
1:B:192:ALA:HB1	1:B:414:GLU:OE2	2.06	0.55
3:D:116:ILE:HD12	3:D:193:CYS:HB3	1.88	0.55
1:B:218:VAL:O	1:B:219:PHE:C	2.44	0.55
2:C:178:LEU:HB2	2:C:183:TYR:HE2	1.71	0.55
1:A:210:TYR:CE1	1:B:208:PHE:HA	2.42	0.55
3:F:132:VAL:HG12	3:F:133:CYS:N	2.22	0.55
2:E:67:LYS:NZ	2:E:85:LYS:O	2.36	0.55
2:C:106:TRP:N	2:C:106:TRP:CD1	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7:SER:OG	3:F:8:PRO:HD3	2.07	0.55
3:F:30:SER:HA	3:F:70:TYR:OH	2.06	0.55
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.41	0.55
2:C:105:TYR:HD2	3:D:30:SER:O	1.89	0.55
1:B:160:ARG:O	1:B:163:LEU:HB3	2.07	0.55
3:D:124:LEU:C	3:D:126:SER:H	2.10	0.55
1:B:287:ASN:HD22	1:B:290:LYS:CG	2.20	0.54
2:C:7:SER:HA	2:C:115:THR:CG2	2.38	0.54
1:B:53:PHE:CE1	1:B:136:LEU:HD12	2.41	0.54
2:E:49:GLY:HA3	2:E:70:ILE:HD11	1.90	0.54
1:B:362:ALA:O	1:B:366:VAL:HG23	2.07	0.54
3:D:29:VAL:HG23	3:D:70:TYR:CE1	2.43	0.54
1:B:169:LYS:HG2	1:B:170:GLY:N	2.22	0.54
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.90	0.54
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.88	0.54
1:A:42:VAL:HG23	1:A:162:VAL:HG21	1.88	0.54
2:E:50:GLU:OE1	3:F:90:TRP:HH2	1.90	0.54
3:F:95:GLN:H	3:F:95:GLN:CD	2.11	0.54
3:F:191:TYR:O	3:F:207:SER:HB2	2.07	0.54
1:A:190:PHE:HD1	1:A:411:LEU:HD11	1.73	0.54
2:E:150:VAL:HB	2:E:185:LEU:HD12	1.90	0.54
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.88	0.54
1:B:444:LEU:O	1:B:444:LEU:HD13	2.08	0.54
2:E:104:GLY:O	2:E:106:TRP:CD1	2.61	0.54
3:F:4:LEU:HD22	3:F:23:CYS:SG	2.48	0.54
3:D:178:LEU:HD12	3:D:179:THR:N	2.23	0.54
2:E:57:THR:C	2:E:58:ILE:HG12	2.28	0.54
1:A:381:GLN:HE21	1:A:381:GLN:H	0.74	0.54
1:B:108:GLY:CA	1:B:153:GLN:NE2	2.70	0.54
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.89	0.54
2:E:107:TYR:CE2	3:F:48:TYR:CD1	2.92	0.54
1:A:320:ILE:HG21	1:A:394:MET:HE1	1.89	0.54
1:B:274:LEU:HD23	1:B:277:GLN:HE22	1.73	0.54
1:A:250:ASN:ND2	2:C:105:TYR:CD1	2.74	0.54
2:E:132:LEU:HD11	2:E:149:LEU:HB2	1.90	0.54
2:C:106:TRP:H	2:C:106:TRP:HD1	1.52	0.54
1:B:33:LEU:HD23	1:B:33:LEU:O	2.08	0.54
3:F:185:TYR:CD1	3:F:191:TYR:CE1	2.96	0.53
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.38	0.53
3:D:139:TYR:O	3:D:172:TYR:HD1	1.91	0.53
1:A:108:GLY:CA	1:A:153:GLN:NE2	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:76:THR:HG22	3:D:76:THR:O	2.08	0.53
3:D:90:TRP:CH2	3:D:95:GLN:NE2	2.76	0.53
3:D:185:TYR:HA	3:D:191:TYR:OH	2.07	0.53
1:B:200:ILE:CG2	1:B:201:ILE:N	2.71	0.53
3:D:139:TYR:HB3	3:D:140:PRO:CD	2.39	0.53
1:B:267:PRO:O	1:B:270:ASN:HB2	2.07	0.53
3:D:90:TRP:CD2	3:D:95:GLN:NE2	2.77	0.53
3:F:145:VAL:HG11	3:F:176:SER:OG	2.08	0.53
3:D:186:GLU:C	3:D:188:HIS:H	2.12	0.53
3:D:192:THR:HA	3:D:207:SER:CB	2.39	0.53
2:C:83:ILE:HD11	2:C:94:TYR:CE1	2.43	0.53
1:A:190:PHE:CD1	1:A:411:LEU:HD21	2.43	0.53
3:D:58:PRO:C	3:D:60:ARG:H	2.12	0.53
1:B:288:ILE:CG2	1:B:289:THR:N	2.72	0.53
3:F:76:THR:HG22	3:F:76:THR:O	2.09	0.53
2:C:185:LEU:CD1	2:C:185:LEU:C	2.77	0.53
3:F:82:ALA:HB2	3:F:105:ILE:HD12	1.90	0.53
3:F:54:THR:HG22	3:F:55:SER:H	1.74	0.53
1:B:144:VAL:HG21	1:B:343:THR:HB	1.90	0.53
1:B:282:ARG:O	1:B:284:HIS:N	2.41	0.53
1:A:308:VAL:O	1:A:309:ALA:HB2	2.08	0.53
3:F:181:THR:OG1	3:F:184:GLU:HB3	2.08	0.53
2:C:41:PRO:C	2:C:43:LYS:H	2.12	0.53
3:F:74:ILE:CG2	3:F:77:MET:HA	2.39	0.53
1:B:108:GLY:HA3	1:B:153:GLN:HE21	1.73	0.53
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.90	0.53
2:C:165:GLY:C	2:C:167:LEU:H	2.12	0.53
1:B:358:ALA:O	1:B:361:LEU:HB2	2.09	0.53
2:C:126:PRO:HA	2:C:210:SER:OG	2.09	0.53
2:C:99:LEU:HD21	2:C:108:PHE:CD2	2.43	0.53
1:A:171:ASP:HB3	1:A:212:LEU:HD13	1.90	0.53
1:A:419:TYR:OH	1:B:414:GLU:HG2	2.08	0.53
2:C:6:GLU:OE2	2:C:96:CYS:N	2.42	0.53
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.91	0.52
3:F:133:CYS:HB2	3:F:147:TRP:HH2	1.74	0.52
3:D:169:ASP:OD1	3:D:171:THR:HG23	2.09	0.52
1:A:31:THR:H	1:B:437:GLN:NE2	2.08	0.52
1:A:437:GLN:HE22	1:B:31:THR:H	1.56	0.52
1:B:99:LYS:HG2	1:B:100:TYR:CE1	2.44	0.52
3:D:19:VAL:O	3:D:73:THR:HG23	2.09	0.52
2:E:87:ARG:HG3	2:E:89:GLU:OE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ILE:HD12	1:B:425:MET:HE3	1.91	0.52
2:E:196:TRP:CD1	2:E:196:TRP:C	2.83	0.52
3:F:132:VAL:HA	3:F:177:THR:HG23	1.90	0.52
3:F:136:ASN:HB3	3:F:137:ASN:HD22	1.75	0.52
3:D:37:GLN:HE21	3:D:43:PRO:HD3	1.73	0.52
2:C:177:VAL:CG2	3:D:159:LEU:CD1	2.86	0.52
1:B:324:THR:HG23	1:B:390:ALA:HB3	1.91	0.52
1:A:419:TYR:CE1	1:B:414:GLU:HG2	2.44	0.52
1:A:422:ILE:HG23	1:A:423:LEU:N	2.24	0.52
3:D:112:PRO:HG2	3:D:204:ILE:CD1	2.38	0.52
1:B:116:LEU:CD2	1:B:178:LEU:HD23	2.37	0.52
1:A:274:LEU:HD23	1:A:277:GLN:NE2	2.24	0.52
3:F:162:TRP:HE3	3:F:162:TRP:N	2.08	0.52
1:A:143:MET:HB3	1:A:347:CYS:SG	2.49	0.52
2:C:174:PHE:CE1	3:D:175:SER:HB3	2.45	0.52
2:C:7:SER:CA	2:C:115:THR:HG21	2.39	0.52
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.45	0.52
3:F:164:ASP:O	3:F:165:GLN:C	2.47	0.52
3:F:29:VAL:HA	3:F:91:SER:OG	2.09	0.52
3:F:29:VAL:HG23	3:F:70:TYR:HE1	1.74	0.52
2:C:194:SER:O	2:C:198:SER:OG	2.26	0.52
1:A:208:PHE:HA	1:B:210:TYR:CE1	2.45	0.52
2:C:45:LEU:HD11	3:D:86:TYR:CE1	2.45	0.52
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.38	0.52
1:A:444:LEU:HD13	1:A:444:LEU:O	2.10	0.52
1:B:249:LEU:C	1:B:251:THR:H	2.12	0.52
2:E:143:MET:SD	2:E:192:PRO:HA	2.49	0.52
3:D:119:PRO:HD3	3:D:131:VAL:HG22	1.92	0.52
2:C:111:TRP:N	2:C:111:TRP:CD1	2.78	0.52
3:D:79:ALA:HB1	3:D:105:ILE:HD11	1.91	0.52
1:B:320:ILE:HD13	1:B:394:MET:HE1	1.89	0.52
3:F:162:TRP:HE3	3:F:162:TRP:H	1.58	0.52
3:F:48:TYR:CD2	3:F:52:LYS:HB2	2.45	0.52
3:D:107:ARG:NH2	3:D:108:ALA:O	2.26	0.52
2:C:6:GLU:CG	2:C:114:GLY:HA2	2.40	0.52
3:D:22:THR:CG2	3:D:23:CYS:H	2.13	0.52
1:A:183:ALA:HB2	1:A:200:ILE:HD13	1.92	0.52
2:E:162:TRP:CD1	2:E:171:VAL:HG13	2.45	0.52
1:A:340:ARG:HA	1:A:343:THR:OG1	2.10	0.52
2:E:151:LYS:HB2	2:E:184:THR:OG1	2.10	0.52
1:A:19:ARG:HB2	1:A:19:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:189:ASN:HD21	3:F:211:ALA:H	1.58	0.51
3:D:167:SER:OG	3:D:168:LYS:HE3	2.10	0.51
2:E:200:THR:O	2:E:200:THR:CG2	2.57	0.51
1:B:148:GLU:OE1	1:B:355:GLY:HA3	2.10	0.51
2:C:145:THR:O	2:C:146:LEU:HD23	2.10	0.51
2:C:163:ASN:O	2:C:164:SER:HB2	2.10	0.51
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.91	0.51
1:B:74:ASN:ND2	1:B:76:PRO:HD2	2.25	0.51
1:A:100:TYR:O	1:A:101:ALA:HB2	2.10	0.51
1:A:65:MET:C	1:A:67:ALA:H	2.14	0.51
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.91	0.51
2:C:161:THR:O	2:C:204:ASN:OD1	2.29	0.51
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.74	0.51
1:A:358:ALA:O	1:A:361:LEU:HB2	2.10	0.51
3:F:131:VAL:HG12	3:F:147:TRP:CZ3	2.45	0.51
3:D:73:THR:HG22	3:D:74:ILE:N	2.25	0.51
1:B:381:GLN:H	1:B:381:GLN:HE21	0.75	0.51
3:F:210:ARG:CB	3:F:210:ARG:NH1	2.68	0.51
2:E:36:TRP:CZ3	2:E:96:CYS:HB3	2.46	0.51
1:A:158:ILE:O	1:A:162:VAL:HG13	2.10	0.51
3:D:131:VAL:HG12	3:D:147:TRP:CH2	2.45	0.51
2:C:6:GLU:HA	2:C:21:SER:O	2.10	0.51
3:F:150:ASP:OD1	3:F:189:ASN:N	2.35	0.51
3:F:48:TYR:HD2	3:F:48:TYR:H	1.57	0.51
1:A:423:LEU:CB	1:A:424:PRO:HD3	2.30	0.51
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.37	0.51
1:A:227:ILE:O	1:A:231:ILE:HG12	2.11	0.51
3:F:48:TYR:CD2	3:F:52:LYS:O	2.64	0.51
1:B:320:ILE:HG21	1:B:394:MET:CE	2.32	0.51
2:C:146:LEU:HB2	2:C:189:VAL:HG12	1.93	0.51
3:F:179:THR:O	3:F:180:LEU:HD23	2.11	0.51
1:A:356:ILE:HG23	1:A:356:ILE:O	2.11	0.51
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.75	0.50
2:E:50:GLU:OE1	3:F:90:TRP:CH2	2.64	0.50
2:E:107:TYR:CB	3:F:33:HIS:CD2	2.85	0.50
3:D:47:ILE:HG13	3:D:53:LEU:CD2	2.41	0.50
3:F:191:TYR:O	3:F:207:SER:CB	2.59	0.50
1:A:208:PHE:N	1:A:208:PHE:CD1	2.80	0.50
2:C:45:LEU:N	2:C:45:LEU:HD12	2.25	0.50
1:B:190:PHE:HD1	1:B:411:LEU:HD11	1.76	0.50
1:A:459:GLU:O	1:A:459:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:148:LYS:HB2	3:F:192:THR:HG1	1.75	0.50
2:E:91:THR:O	2:E:92:ALA:HB2	2.11	0.50
2:E:125:THR:O	2:E:153:TYR:HA	2.11	0.50
2:E:18:LEU:CD2	2:E:18:LEU:N	2.75	0.50
2:C:192:PRO:O	2:C:195:SER:CB	2.59	0.50
1:A:75:TYR:HB3	1:A:76:PRO:CD	2.36	0.50
3:F:162:TRP:CE3	3:F:162:TRP:N	2.79	0.50
1:A:117:GLU:O	1:A:118:ASP:HB2	2.11	0.50
3:D:3:VAL:O	3:D:3:VAL:HG12	2.11	0.50
1:A:27:GLU:OE1	1:A:27:GLU:HA	2.11	0.50
1:A:116:LEU:HD12	1:A:204:MET:O	2.12	0.50
3:D:132:VAL:HG22	3:D:177:THR:HG23	1.92	0.50
1:A:148:GLU:O	1:A:149:GLY:C	2.50	0.50
2:E:29:TYR:CD2	2:E:77:ASP:HA	2.46	0.50
3:D:123:GLN:HE22	3:D:130:SER:CB	2.25	0.50
2:E:129:VAL:HG21	2:E:214:VAL:HG23	1.94	0.50
1:A:234:HIS:HE1	3:F:52:LYS:HZ3	1.59	0.50
1:A:17:ARG:O	1:A:20:GLN:HB3	2.12	0.50
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.93	0.50
3:F:159:LEU:O	3:F:176:SER:HA	2.12	0.50
1:A:273:VAL:HG11	1:A:444:LEU:HD21	1.93	0.50
3:F:164:ASP:OD2	3:F:165:GLN:N	2.44	0.50
2:C:19:LYS:HG3	2:C:82:GLN:HG2	1.93	0.50
1:B:74:ASN:HD21	1:B:76:PRO:HD2	1.77	0.50
3:F:124:LEU:C	3:F:126:SER:H	2.15	0.50
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.94	0.50
1:A:120:ARG:NH1	1:A:452:THR:CG2	2.75	0.50
1:A:383:HIS:HD2	2:C:33:TRP:CZ3	2.30	0.50
1:A:241:VAL:HG12	1:A:241:VAL:O	2.11	0.50
1:B:117:GLU:O	1:B:118:ASP:HB2	2.11	0.50
1:A:131:LYS:CE	1:A:150:PRO:HA	2.40	0.50
1:A:218:VAL:O	1:A:219:PHE:C	2.49	0.50
1:B:148:GLU:O	1:B:149:GLY:C	2.47	0.50
3:F:56:GLY:O	3:F:57:VAL:C	2.49	0.50
2:E:93:LEU:HD12	2:E:115:THR:O	2.12	0.50
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.47	0.50
3:F:48:TYR:HD2	3:F:48:TYR:N	2.10	0.50
3:D:79:ALA:C	3:D:81:ASP:H	2.14	0.50
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.30	0.50
1:A:284:HIS:HA	1:A:290:LYS:HB3	1.94	0.50
2:C:163:ASN:O	2:C:164:SER:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:46:TRP:HE3	3:D:46:TRP:HA	1.76	0.50
1:B:356:ILE:O	1:B:356:ILE:HG23	2.11	0.50
1:A:288:ILE:CG2	1:A:289:THR:N	2.74	0.50
2:E:150:VAL:HB	2:E:185:LEU:CD1	2.41	0.49
2:C:175:PRO:HD2	3:D:161:SER:OG	2.12	0.49
1:B:279:LEU:O	1:B:279:LEU:HD23	2.12	0.49
1:A:97:VAL:HG22	1:A:104:ALA:HB3	1.94	0.49
1:A:241:VAL:CG1	1:A:244:LEU:HD21	2.34	0.49
2:C:162:TRP:C	2:C:164:SER:H	2.15	0.49
2:E:68:PHE:HD2	2:E:83:ILE:HG23	1.76	0.49
2:E:40:ALA:HA	2:E:92:ALA:CB	2.42	0.49
3:F:150:ASP:OD2	3:F:188:HIS:CB	2.61	0.49
2:C:129:VAL:CG2	2:C:214:VAL:HG21	2.39	0.49
3:D:107:ARG:HG3	3:D:139:TYR:CD2	2.47	0.49
2:C:200:THR:CG2	2:C:200:THR:O	2.60	0.49
2:E:131:PRO:CB	2:E:218:ILE:HD13	2.43	0.49
2:C:108:PHE:CD1	3:D:97:PHE:HZ	2.30	0.49
2:E:93:LEU:HD11	2:E:114:GLY:HA3	1.94	0.49
2:E:52:ASN:O	2:E:52:ASN:OD1	2.30	0.49
3:D:205:VAL:O	3:D:206:LYS:HG2	2.12	0.49
2:E:106:TRP:CD1	2:E:106:TRP:N	2.80	0.49
1:B:74:ASN:HD22	1:B:74:ASN:C	2.15	0.49
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.94	0.49
1:B:198:LEU:HD12	1:B:406:LEU:HG	1.94	0.49
1:A:348:PHE:CD1	1:A:356:ILE:HB	2.48	0.49
3:D:66:SER:O	3:D:68:THR:N	2.45	0.49
1:B:44:THR:O	1:B:48:LEU:HG	2.12	0.49
3:F:48:TYR:N	3:F:48:TYR:CD2	2.80	0.49
3:F:88:GLN:CB	3:F:97:PHE:CD1	2.91	0.49
3:F:150:ASP:OD2	3:F:188:HIS:ND1	2.46	0.49
1:A:208:PHE:O	1:A:209:ARG:CB	2.59	0.49
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.94	0.49
1:B:308:VAL:O	1:B:309:ALA:HB2	2.13	0.49
1:A:274:LEU:O	1:A:277:GLN:HB2	2.13	0.49
2:E:93:LEU:CD1	2:E:115:THR:H	2.25	0.49
1:B:235:GLU:O	1:B:236:VAL:CG2	2.61	0.49
1:A:18:ARG:HB2	1:B:119:GLN:OE1	2.13	0.49
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.38	0.49
3:D:151:GLY:O	3:D:152:SER:HB2	2.13	0.49
3:D:185:TYR:HD1	3:D:191:TYR:CZ	2.31	0.48
2:C:196:TRP:HD1	2:C:201:VAL:HG23	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:SER:O	1:B:340:ARG:NH2	2.46	0.48
3:D:184:GLU:HA	3:D:187:ARG:NH1	2.28	0.48
3:F:191:TYR:CB	3:F:208:PHE:CE2	2.96	0.48
2:C:196:TRP:HB3	2:C:197:PRO:HD3	1.95	0.48
3:D:172:TYR:O	3:D:173:SER:OG	2.31	0.48
1:B:309:ALA:O	1:B:311:ALA:N	2.45	0.48
1:B:148:GLU:HG2	1:B:357:PHE:CD2	2.48	0.48
1:A:320:ILE:HG21	1:A:394:MET:CE	2.43	0.48
3:D:139:TYR:O	3:D:172:TYR:CD1	2.66	0.48
2:E:191:VAL:HB	2:E:192:PRO:CD	2.43	0.48
2:E:131:PRO:HD3	2:E:216:LYS:CG	2.42	0.48
3:D:153:GLU:HG3	3:D:154:ARG:N	2.27	0.48
3:D:1:ASP:O	3:D:1:ASP:OD1	2.30	0.48
1:A:380:PRO:HG2	3:D:93:HIS:HB2	1.96	0.48
1:A:127:VAL:HB	1:A:157:ASN:HD21	1.77	0.48
1:B:294:MET:HG2	1:B:294:MET:O	2.14	0.48
2:C:11:LEU:CD1	2:C:154:PHE:HE2	2.26	0.48
2:E:51:ILE:O	2:E:51:ILE:HG23	2.13	0.48
3:F:194:GLU:OE1	3:F:203:PRO:HB2	2.12	0.48
2:E:125:THR:O	2:E:125:THR:HG22	2.13	0.48
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.96	0.48
1:A:416:THR:O	1:A:418:ASN:ND2	2.42	0.48
1:A:383:HIS:NE2	3:D:90:TRP:CZ2	2.81	0.48
3:D:90:TRP:O	3:D:90:TRP:CD1	2.66	0.48
1:A:282:ARG:O	1:A:284:HIS:N	2.47	0.48
3:F:29:VAL:HG23	3:F:70:TYR:CE1	2.48	0.48
2:E:49:GLY:HA3	2:E:70:ILE:CD1	2.43	0.48
1:B:100:TYR:O	1:B:101:ALA:HB2	2.13	0.48
1:B:190:PHE:CD1	1:B:411:LEU:HD11	2.49	0.48
1:B:235:GLU:O	1:B:236:VAL:HG23	2.13	0.48
1:A:362:ALA:O	1:A:366:VAL:HG23	2.14	0.48
1:A:83:PHE:CD1	1:A:83:PHE:C	2.86	0.48
3:D:38:LYS:O	3:D:39:SER:C	2.51	0.48
1:B:443:PRO:O	1:B:445:TYR:N	2.46	0.48
3:D:181:THR:O	3:D:182:LYS:C	2.52	0.48
2:C:32:TYR:HE2	2:C:98:ARG:CD	2.26	0.48
1:A:273:VAL:HA	1:A:345:LEU:HD22	1.94	0.48
1:A:313:SER:OG	1:A:314:GLY:N	2.47	0.48
1:A:148:GLU:HG2	1:A:357:PHE:HD2	1.79	0.48
2:C:174:PHE:CD1	3:D:175:SER:HB3	2.48	0.48
3:F:123:GLN:HE22	3:F:130:SER:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:HB3	1:B:299:GLY:O	2.13	0.48
1:B:64:ARG:O	1:B:67:ALA:HB3	2.14	0.48
3:F:189:ASN:HA	3:F:210:ARG:HD3	1.94	0.48
3:F:17:ASP:O	3:F:76:THR:HA	2.13	0.48
3:D:33:HIS:HB2	3:D:88:GLN:OE1	2.13	0.48
3:D:137:ASN:ND2	3:D:137:ASN:N	2.62	0.48
1:A:18:ARG:O	1:A:22:ILE:HG13	2.14	0.48
1:A:75:TYR:O	1:A:78:LEU:HB3	2.14	0.48
2:E:87:ARG:HG3	2:E:89:GLU:H	1.79	0.48
1:B:128:LEU:HD21	1:B:157:ASN:HB2	1.94	0.48
1:B:83:PHE:CD1	1:B:84:LEU:HD23	2.49	0.48
1:B:224:MET:O	1:B:228:MET:HG2	2.14	0.48
2:C:53:PRO:O	2:C:74:ASN:ND2	2.43	0.47
2:E:127:PRO:HB2	2:E:150:VAL:HG12	1.95	0.47
1:B:422:ILE:HG23	1:B:423:LEU:N	2.29	0.47
1:B:305:LEU:C	1:B:307:PHE:H	2.17	0.47
2:E:179:GLN:O	2:E:180:ALA:CB	2.62	0.47
1:A:189:ALA:O	1:A:190:PHE:HD2	1.98	0.47
2:C:177:VAL:O	2:C:177:VAL:HG23	2.14	0.47
2:C:189:VAL:O	2:C:189:VAL:HG13	2.13	0.47
1:B:410:ILE:O	1:B:414:GLU:HB2	2.13	0.47
3:F:192:THR:CB	3:F:207:SER:HB3	2.43	0.47
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.49	0.47
2:C:185:LEU:HD12	2:C:185:LEU:C	2.35	0.47
3:D:149:ILE:HD11	3:D:178:LEU:HD21	1.96	0.47
3:D:116:ILE:HG21	3:D:206:LYS:O	2.15	0.47
2:C:131:PRO:HD3	2:C:216:LYS:HD2	1.96	0.47
1:A:454:ALA:C	1:A:456:GLN:H	2.17	0.47
3:F:72:LEU:CD2	3:F:72:LEU:C	2.83	0.47
3:F:150:ASP:OD2	3:F:188:HIS:HA	2.14	0.47
2:C:147:GLY:CA	2:C:162:TRP:HH2	2.22	0.47
3:D:13:ALA:CB	3:D:77:MET:HE3	2.38	0.47
1:A:320:ILE:N	1:A:321:PRO:CD	2.78	0.47
2:E:132:LEU:HB3	3:F:117:PHE:CD2	2.49	0.47
1:B:274:LEU:HD23	1:B:277:GLN:NE2	2.30	0.47
3:D:7:SER:CB	3:D:8:PRO:CD	2.91	0.47
2:C:178:LEU:HD22	2:C:183:TYR:CZ	2.49	0.47
3:D:150:ASP:OD2	3:D:188:HIS:HB3	2.13	0.47
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.95	0.47
1:A:437:GLN:NE2	1:B:30:LYS:HA	2.29	0.47
3:D:139:TYR:HD1	3:D:140:PRO:HD3	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:20:THR:HG23	3:F:73:THR:HG1	1.77	0.47
1:A:409:ILE:CD1	1:A:426:ILE:HG12	2.44	0.47
1:A:18:ARG:O	1:A:18:ARG:HG2	2.12	0.47
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.96	0.47
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.48	0.47
2:E:24:ALA:HB1	2:E:27:PHE:HE1	1.80	0.47
2:E:27:PHE:HE2	2:E:98:ARG:HG3	1.79	0.47
3:D:143:ILE:HG23	3:D:174:MET:HE1	1.96	0.47
1:A:270:ASN:ND2	1:A:444:LEU:HD23	2.29	0.47
3:F:59:VAL:HG12	3:F:59:VAL:O	2.14	0.47
1:A:457:GLU:OE2	1:B:19:ARG:HD3	2.14	0.47
3:F:75:ASN:O	3:F:76:THR:HB	2.14	0.47
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.97	0.47
3:F:1:ASP:OD1	3:F:1:ASP:N	2.42	0.47
3:F:48:TYR:CE2	3:F:52:LYS:CB	2.96	0.47
3:D:136:ASN:C	3:D:137:ASN:HD22	2.17	0.47
2:E:176:ALA:HA	2:E:185:LEU:HB3	1.95	0.47
2:C:125:THR:HA	2:C:126:PRO:HD2	1.56	0.47
1:B:220:ILE:O	1:B:224:MET:HG2	2.15	0.47
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.96	0.47
3:F:60:ARG:HD3	3:F:78:GLU:HG2	1.97	0.46
1:A:53:PHE:CE1	1:A:136:LEU:HD12	2.50	0.46
2:C:167:LEU:C	2:C:167:LEU:HD12	2.35	0.46
2:C:203:CYS:SG	2:C:203:CYS:O	2.72	0.46
3:F:110:ALA:HB3	3:F:139:TYR:CB	2.45	0.46
2:E:87:ARG:O	2:E:119:VAL:HG21	2.15	0.46
2:E:36:TRP:CE3	2:E:96:CYS:HB3	2.50	0.46
2:C:126:PRO:CA	2:C:210:SER:OG	2.62	0.46
3:F:183:ASP:O	3:F:185:TYR:N	2.48	0.46
3:D:179:THR:O	3:D:180:LEU:HD23	2.16	0.46
1:B:148:GLU:HG2	1:B:357:PHE:HD2	1.79	0.46
3:D:60:ARG:HH11	3:D:81:ASP:CG	2.18	0.46
1:A:182:ALA:HB1	1:A:204:MET:CE	2.46	0.46
1:A:176:THR:HG22	1:A:177:LEU:N	2.30	0.46
1:B:114:GLY:O	1:B:117:GLU:N	2.44	0.46
2:C:174:PHE:CE1	3:D:175:SER:N	2.82	0.46
2:E:30:SER:C	2:E:32:TYR:H	2.18	0.46
3:D:143:ILE:HG23	3:D:174:MET:HE3	1.96	0.46
2:C:134:PRO:O	2:C:221:ARG:HG3	2.16	0.46
2:C:136:SER:C	2:C:138:ALA:H	2.19	0.46
1:B:250:ASN:HB2	2:E:105:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:O	3:D:8:PRO:C	2.53	0.46
2:C:150:VAL:HB	2:C:185:LEU:HD11	1.97	0.46
1:A:248:PRO:HG3	2:C:101:TYR:CZ	2.50	0.46
2:E:6:GLU:H	2:E:6:GLU:CD	2.18	0.46
1:B:269:PHE:O	1:B:273:VAL:HG12	2.15	0.46
2:C:126:PRO:HB3	2:C:210:SER:OG	2.15	0.46
1:A:148:GLU:HG2	1:A:357:PHE:CD2	2.51	0.46
3:D:109:ASP:HA	3:D:139:TYR:HB3	1.98	0.46
2:C:6:GLU:CD	2:C:114:GLY:HA2	2.36	0.46
1:A:437:GLN:NE2	1:B:31:THR:H	2.14	0.46
2:E:67:LYS:HE2	2:E:84:SER:O	2.16	0.46
2:C:67:LYS:HA	2:C:67:LYS:HD3	1.69	0.46
2:C:32:TYR:CE2	2:C:98:ARG:CD	2.99	0.46
1:B:423:LEU:HB3	1:B:424:PRO:CD	2.44	0.46
1:A:83:PHE:CD1	1:A:84:LEU:HD23	2.50	0.46
3:F:89:GLN:HE21	3:F:96:THR:N	2.13	0.45
1:A:422:ILE:CG2	1:A:423:LEU:N	2.78	0.45
3:D:190:SER:O	3:D:191:TYR:CD1	2.69	0.45
3:F:120:SER:OG	3:F:123:GLN:HB2	2.15	0.45
1:A:232:PHE:N	1:A:232:PHE:CD1	2.84	0.45
3:F:32:ILE:HD13	3:F:89:GLN:HB3	1.94	0.45
3:D:47:ILE:HD11	3:D:61:PHE:HB3	1.97	0.45
1:A:74:ASN:C	1:A:74:ASN:HD22	2.18	0.45
1:B:116:LEU:HD12	1:B:204:MET:O	2.16	0.45
1:A:25:LEU:HD23	1:B:208:PHE:CZ	2.51	0.45
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.97	0.45
3:D:116:ILE:HG23	3:D:116:ILE:O	2.16	0.45
1:B:83:PHE:CD1	1:B:83:PHE:C	2.89	0.45
1:B:312:THR:HG22	1:B:339:ALA:CB	2.46	0.45
3:D:47:ILE:HD13	3:D:72:LEU:HD12	1.98	0.45
1:B:163:LEU:HD22	1:B:174:ARG:HA	1.98	0.45
2:C:32:TYR:CD2	2:C:98:ARG:CG	2.99	0.45
1:A:361:LEU:HD23	1:A:394:MET:O	2.15	0.45
1:B:422:ILE:CG2	1:B:423:LEU:N	2.79	0.45
3:D:139:TYR:O	3:D:140:PRO:C	2.53	0.45
1:B:357:PHE:CE1	1:B:398:LEU:HD22	2.51	0.45
2:E:178:LEU:HD12	2:E:182:LEU:O	2.16	0.45
2:E:210:SER:O	2:E:211:SER:HB3	2.17	0.45
3:F:183:ASP:O	3:F:186:GLU:N	2.50	0.45
2:C:130:TYR:HB3	3:D:120:SER:HG	1.81	0.45
1:A:30:LYS:HA	1:B:437:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:PHE:CG	3:F:175:SER:HB3	2.51	0.45
3:F:48:TYR:HD2	3:F:52:LYS:O	1.99	0.45
1:B:402:ILE:CG1	1:B:402:ILE:O	2.64	0.45
2:E:35:SER:HB2	2:E:49:GLY:O	2.16	0.45
1:A:68:LEU:CD2	1:A:81:VAL:HG23	2.47	0.45
1:B:385:GLU:O	1:B:386:ALA:C	2.55	0.45
3:F:138:PHE:CD1	3:F:140:PRO:O	2.69	0.45
1:B:284:HIS:HB3	1:B:290:LYS:O	2.17	0.45
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.81	0.45
2:E:16:GLY:N	2:E:86:VAL:HG22	2.25	0.45
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.99	0.45
3:F:185:TYR:CE1	3:F:191:TYR:HE1	2.34	0.45
2:C:105:TYR:CE2	3:D:31:TYR:CD1	3.01	0.45
1:B:171:ASP:CB	1:B:212:LEU:HD22	2.39	0.45
1:B:312:THR:HG22	1:B:339:ALA:HB3	1.98	0.45
2:E:38:ARG:HE	2:E:46:LYS:HE3	1.81	0.45
1:B:399:ALA:O	1:B:403:ARG:HA	2.16	0.45
1:B:127:VAL:CB	1:B:157:ASN:HD21	2.27	0.45
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.52	0.45
1:A:42:VAL:CG2	1:A:162:VAL:HG21	2.46	0.45
2:E:108:PHE:HD1	3:F:88:GLN:NE2	2.11	0.45
2:C:104:GLY:C	2:C:105:TYR:HD1	2.19	0.45
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.32	0.45
2:E:18:LEU:HD11	2:E:117:VAL:HG11	1.99	0.45
1:B:131:LYS:HE2	1:B:153:GLN:HE21	1.80	0.45
3:D:1:ASP:O	3:D:1:ASP:CG	2.55	0.45
3:F:5:THR:O	3:F:5:THR:HG22	2.16	0.45
1:B:270:ASN:O	1:B:273:VAL:CG1	2.65	0.45
1:B:228:MET:O	1:B:232:PHE:HD1	2.00	0.45
3:D:197:HIS:CE1	3:D:199:THR:HG23	2.52	0.45
1:B:68:LEU:CD2	1:B:81:VAL:HG23	2.47	0.45
3:F:210:ARG:CG	3:F:210:ARG:NH1	2.70	0.44
2:C:150:VAL:HB	2:C:185:LEU:HD12	1.99	0.44
2:E:95:TYR:OH	3:F:37:GLN:NE2	2.50	0.44
3:F:131:VAL:HG12	3:F:147:TRP:CH2	2.52	0.44
1:B:54:ASP:OD1	1:B:147:ARG:NE	2.45	0.44
1:B:42:VAL:HG23	1:B:162:VAL:HG21	1.97	0.44
2:C:33:TRP:CE2	2:C:52:ASN:HB3	2.52	0.44
2:E:18:LEU:HD11	2:E:117:VAL:CG1	2.47	0.44
1:A:124:TRP:HB3	1:A:157:ASN:HB3	1.99	0.44
3:D:114:VAL:HG11	3:D:206:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:THR:O	1:A:417:ASP:C	2.56	0.44
3:D:58:PRO:CB	3:D:60:ARG:NH2	2.81	0.44
3:D:19:VAL:O	3:D:73:THR:HA	2.18	0.44
3:F:191:TYR:CB	3:F:208:PHE:HE2	2.30	0.44
3:F:34:TRP:CE3	3:F:87:CYS:HB3	2.53	0.44
3:F:111:ALA:CA	3:F:199:THR:HG21	2.46	0.44
1:A:413:LEU:HD22	1:A:422:ILE:HD13	1.98	0.44
2:E:98:ARG:O	2:E:109:ASP:HB3	2.18	0.44
1:B:236:VAL:HG12	1:B:237:ALA:N	2.33	0.44
2:C:13:GLN:HA	2:C:120:SER:O	2.18	0.44
1:A:234:HIS:HE1	3:F:52:LYS:NZ	2.09	0.44
3:F:88:GLN:HG3	3:F:97:PHE:CD1	2.52	0.44
1:A:380:PRO:HG2	3:D:93:HIS:CB	2.47	0.44
1:A:190:PHE:CE1	1:A:411:LEU:HD21	2.52	0.44
1:A:231:ILE:HB	1:A:232:PHE:CD1	2.53	0.44
1:B:190:PHE:HD1	1:B:411:LEU:CD1	2.31	0.44
2:E:29:TYR:HB2	2:E:77:ASP:OD2	2.17	0.44
1:A:267:PRO:O	1:A:270:ASN:HB2	2.17	0.44
2:E:122:ALA:HB3	2:E:154:PHE:CE2	2.52	0.44
3:F:185:TYR:CE1	3:F:191:TYR:CE1	3.06	0.44
1:B:287:ASN:HD22	1:B:290:LYS:N	2.11	0.44
2:C:105:TYR:CD1	2:C:105:TYR:N	2.86	0.44
3:D:124:LEU:HD22	3:D:182:LYS:HG3	2.00	0.44
1:B:422:ILE:HA	1:B:425:MET:HE2	2.00	0.44
1:B:340:ARG:HA	1:B:343:THR:OG1	2.17	0.44
2:E:175:PRO:HG2	3:F:162:TRP:O	2.18	0.44
2:C:11:LEU:HD11	2:C:154:PHE:HE2	1.82	0.44
2:E:52:ASN:C	2:E:52:ASN:OD1	2.56	0.44
3:F:66:SER:N	3:F:70:TYR:CE2	2.85	0.44
2:C:162:TRP:C	2:C:164:SER:N	2.69	0.44
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.99	0.44
1:A:270:ASN:CG	1:A:444:LEU:HD23	2.38	0.44
3:F:109:ASP:OD1	3:F:198:LYS:HE2	2.18	0.44
1:B:287:ASN:HD22	1:B:290:LYS:CB	2.30	0.44
3:D:50:THR:CG2	3:D:70:TYR:CD2	3.00	0.44
1:B:209:ARG:HG3	1:B:210:TYR:O	2.17	0.44
1:A:249:LEU:C	1:A:251:THR:N	2.69	0.44
2:C:151:LYS:HG3	2:C:152:GLY:N	2.33	0.44
3:D:73:THR:CG2	3:D:74:ILE:N	2.80	0.44
2:C:176:ALA:HA	2:C:185:LEU:HB3	2.00	0.44
1:B:405:PRO:HG2	1:B:406:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ALA:O	1:B:189:ALA:N	2.51	0.44
2:C:64:LEU:O	2:C:65:LYS:C	2.55	0.44
3:F:4:LEU:HA	3:F:24:SER:O	2.18	0.43
1:B:239:ILE:HD13	1:B:394:MET:HE1	2.00	0.43
2:E:134:PRO:O	2:E:221:ARG:HG3	2.17	0.43
1:B:90:ALA:CB	1:B:299:GLY:HA3	2.48	0.43
2:C:138:ALA:O	2:C:140:ALA:N	2.49	0.43
1:A:44:THR:O	1:A:48:LEU:HG	2.18	0.43
3:F:185:TYR:HD1	3:F:191:TYR:CE1	2.36	0.43
1:B:27:GLU:HA	1:B:27:GLU:OE1	2.18	0.43
2:C:108:PHE:CE1	3:D:97:PHE:CZ	3.06	0.43
2:E:48:ILE:HD13	2:E:48:ILE:N	2.34	0.43
2:E:210:SER:OG	2:E:212:THR:HG23	2.18	0.43
3:D:61:PHE:HA	3:D:73:THR:O	2.17	0.43
2:E:172:HIS:CD2	3:F:173:SER:OG	2.71	0.43
2:C:132:LEU:HD11	2:C:149:LEU:HB2	1.99	0.43
1:A:128:LEU:HD21	1:A:157:ASN:HB2	1.98	0.43
2:C:7:SER:C	2:C:115:THR:HG21	2.38	0.43
2:C:78:THR:HG22	2:C:79:LEU:N	2.32	0.43
1:B:378:LEU:HB2	1:B:379:PHE:CE1	2.54	0.43
3:F:88:GLN:HG2	3:F:89:GLN:N	2.33	0.43
3:F:185:TYR:CD1	3:F:191:TYR:HE1	2.35	0.43
3:D:189:ASN:HD21	3:D:209:ASN:HB3	1.83	0.43
3:F:119:PRO:HG3	3:F:130:SER:C	2.39	0.43
1:B:279:LEU:HD23	1:B:279:LEU:C	2.39	0.43
3:D:30:SER:O	3:D:31:TYR:HB2	2.18	0.43
1:B:320:ILE:N	1:B:321:PRO:CD	2.81	0.43
1:B:171:ASP:HB3	1:B:212:LEU:HD13	1.99	0.43
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.52	0.43
3:D:117:PHE:HA	3:D:118:PRO:HD3	1.92	0.43
3:D:192:THR:HB	3:D:207:SER:HB3	2.00	0.43
3:D:133:CYS:HB2	3:D:147:TRP:CH2	2.54	0.43
1:A:422:ILE:HD12	1:A:425:MET:HE3	2.00	0.43
1:B:320:ILE:O	1:B:324:THR:OG1	2.34	0.43
2:C:196:TRP:C	2:C:198:SER:N	2.71	0.43
1:B:423:LEU:O	1:B:427:ILE:HG13	2.18	0.43
3:D:138:PHE:HE1	3:D:141:LYS:HA	1.84	0.43
1:A:255:TYR:O	1:A:428:THR:HA	2.18	0.43
2:E:177:VAL:HG21	3:F:159:LEU:HD13	2.00	0.43
3:F:194:GLU:OE1	3:F:203:PRO:CB	2.67	0.43
1:B:180:THR:O	1:B:181:GLY:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:TYR:HD2	1:B:445:TYR:HA	1.72	0.43
1:A:124:TRP:CB	1:A:157:ASN:HB3	2.49	0.43
1:A:430:LEU:HD21	1:B:220:ILE:CG1	2.48	0.43
2:C:112:GLY:O	3:D:42:SER:CB	2.66	0.43
2:E:52:ASN:HB2	2:E:53:PRO:HD2	2.00	0.43
3:F:32:ILE:HG23	3:F:88:GLN:O	2.18	0.43
3:D:18:LYS:HG3	3:D:75:ASN:HA	2.00	0.43
3:D:58:PRO:O	3:D:60:ARG:N	2.51	0.43
3:F:124:LEU:O	3:F:126:SER:N	2.49	0.43
2:E:144:VAL:HG22	2:E:146:LEU:CD2	2.48	0.43
2:E:139:ALA:O	2:E:141:ALA:N	2.52	0.43
2:E:111:TRP:CD1	2:E:111:TRP:N	2.87	0.43
3:F:113:THR:HG22	3:F:113:THR:O	2.19	0.43
3:F:187:ARG:HG2	3:F:188:HIS:HD2	1.78	0.43
1:A:288:ILE:HG23	1:A:289:THR:N	2.33	0.43
2:E:156:GLU:HA	2:E:157:PRO:HA	1.80	0.43
1:A:324:THR:HG23	1:A:390:ALA:HB3	2.01	0.43
2:C:162:TRP:CZ2	2:C:189:VAL:HB	2.53	0.43
3:D:46:TRP:O	3:D:54:THR:OG1	2.27	0.43
1:A:208:PHE:CZ	1:B:25:LEU:HD23	2.54	0.43
1:A:42:VAL:O	1:A:46:VAL:HG23	2.19	0.43
1:A:30:LYS:HB3	1:A:30:LYS:HE2	1.87	0.43
1:B:251:THR:HG22	1:B:255:TYR:HE1	1.84	0.43
1:B:348:PHE:CD1	1:B:356:ILE:HB	2.54	0.43
2:E:107:TYR:C	2:E:107:TYR:HD1	2.23	0.42
1:A:250:ASN:ND2	2:C:104:GLY:O	2.50	0.42
1:A:421:LEU:O	1:A:424:PRO:HD2	2.19	0.42
1:B:38:MET:O	1:B:41:VAL:HG12	2.18	0.42
2:C:149:LEU:HD22	3:D:132:VAL:CG2	2.49	0.42
1:A:220:ILE:HG12	1:B:430:LEU:HD21	2.00	0.42
1:B:130:VAL:O	1:B:134:GLY:N	2.52	0.42
1:B:250:ASN:CB	2:E:105:TYR:HE1	2.32	0.42
1:A:245:SER:O	1:A:420:GLN:NE2	2.50	0.42
3:D:75:ASN:O	3:D:76:THR:HB	2.19	0.42
3:D:60:ARG:NH1	3:D:81:ASP:OD1	2.52	0.42
3:F:58:PRO:C	3:F:60:ARG:H	2.22	0.42
1:A:409:ILE:HD13	1:A:426:ILE:CG1	2.47	0.42
1:B:117:GLU:HA	1:B:209:ARG:HH12	1.84	0.42
3:D:194:GLU:HG2	3:D:205:VAL:HG12	2.00	0.42
1:A:83:PHE:HD1	1:A:84:LEU:N	2.18	0.42
2:C:171:VAL:O	2:C:171:VAL:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:ILE:CG1	3:D:53:LEU:HD23	2.48	0.42
2:C:32:TYR:HE2	2:C:98:ARG:NE	2.17	0.42
3:F:124:LEU:HA	3:F:128:GLY:O	2.19	0.42
1:A:91:MET:C	1:A:93:GLY:N	2.72	0.42
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.54	0.42
1:A:101:ALA:O	1:A:103:GLU:N	2.52	0.42
1:A:99:LYS:O	1:A:99:LYS:HG3	2.20	0.42
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.19	0.42
1:B:97:VAL:HG22	1:B:104:ALA:HB3	2.01	0.42
3:D:60:ARG:HD3	3:D:76:THR:O	2.19	0.42
3:D:189:ASN:ND2	3:D:211:ALA:H	2.17	0.42
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.02	0.42
1:A:103:GLU:HB3	1:A:111:GLU:HG2	2.01	0.42
1:A:385:GLU:O	1:A:386:ALA:C	2.58	0.42
1:B:120:ARG:NH1	1:B:452:THR:CG2	2.82	0.42
3:F:77:MET:CG	3:F:78:GLU:N	2.80	0.42
1:A:443:PRO:O	1:A:445:TYR:N	2.53	0.42
1:B:128:LEU:HD21	1:B:157:ASN:CB	2.49	0.42
1:B:270:ASN:HA	1:B:273:VAL:CG1	2.48	0.42
2:E:66:ASP:O	2:E:67:LYS:C	2.55	0.42
2:E:57:THR:O	2:E:58:ILE:HG12	2.18	0.42
2:E:208:PRO:O	2:E:209:ALA:C	2.58	0.42
2:E:4:LEU:HA	2:E:4:LEU:HD12	1.94	0.42
3:D:2:ILE:HG21	3:D:29:VAL:CG1	2.50	0.42
1:A:216:LYS:HD3	1:B:434:LEU:CD2	2.49	0.42
1:A:38:MET:CA	1:A:41:VAL:HG12	2.44	0.42
1:A:172:GLU:HA	1:A:212:LEU:O	2.19	0.42
3:D:178:LEU:HD12	3:D:179:THR:H	1.83	0.42
3:D:118:PRO:HB3	3:D:208:PHE:CZ	2.55	0.42
2:C:99:LEU:HD21	2:C:108:PHE:CE2	2.55	0.42
3:F:4:LEU:HD12	3:F:96:THR:O	2.20	0.42
3:F:111:ALA:HA	3:F:112:PRO:HD2	1.91	0.42
3:F:119:PRO:HG3	3:F:130:SER:O	2.20	0.42
1:A:31:THR:HA	1:A:32:PRO:HD3	1.95	0.42
2:E:104:GLY:O	2:E:106:TRP:HD1	2.02	0.42
1:A:19:ARG:HB2	1:A:19:ARG:HH11	1.84	0.42
1:B:266:GLY:HA3	1:B:400:ALA:HB1	2.02	0.42
3:D:79:ALA:HB1	3:D:105:ILE:HD13	2.02	0.42
1:B:135:GLY:O	1:B:136:LEU:C	2.58	0.42
1:A:234:HIS:CE1	3:F:52:LYS:HZ3	2.32	0.42
3:D:20:THR:HG23	3:D:73:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:79:ALA:CA	3:D:105:ILE:HD11	2.49	0.42
3:F:150:ASP:OD2	3:F:188:HIS:HB3	2.20	0.42
1:A:249:LEU:O	1:A:251:THR:N	2.53	0.42
1:B:311:ALA:HB1	1:B:336:ILE:HD13	2.01	0.42
2:E:174:PHE:HA	2:E:175:PRO:HD3	1.96	0.42
1:B:43:GLY:O	1:B:44:THR:C	2.57	0.42
1:B:83:PHE:HD1	1:B:84:LEU:HD23	1.85	0.42
1:B:397:LEU:C	1:B:399:ALA:N	2.71	0.42
2:E:173:THR:O	3:F:163:THR:HG22	2.19	0.42
3:F:48:TYR:O	3:F:49:ASP:C	2.58	0.42
1:A:210:TYR:HE1	1:B:208:PHE:HA	1.84	0.42
1:A:305:LEU:C	1:A:307:PHE:H	2.22	0.42
2:C:108:PHE:N	3:D:35:TYR:OH	2.43	0.42
3:F:3:VAL:O	3:F:3:VAL:HG12	2.19	0.42
3:F:77:MET:HG3	3:F:78:GLU:N	2.35	0.41
2:E:29:TYR:O	2:E:32:TYR:HB2	2.19	0.41
1:B:272:TRP:HB3	1:B:345:LEU:CD1	2.49	0.41
2:C:165:GLY:C	2:C:167:LEU:N	2.73	0.41
1:A:107:SER:HB2	1:A:348:PHE:CZ	2.55	0.41
2:C:60:TYR:CD1	2:C:60:TYR:N	2.88	0.41
3:F:49:ASP:O	3:F:51:SER:N	2.51	0.41
2:E:146:LEU:CD2	2:E:146:LEU:N	2.80	0.41
3:D:168:LYS:C	3:D:170:SER:H	2.23	0.41
3:F:192:THR:HG22	3:F:207:SER:HB3	2.00	0.41
1:B:182:ALA:HB3	1:B:200:ILE:HD11	2.03	0.41
1:B:435:LEU:HD13	1:B:435:LEU:HA	1.87	0.41
3:D:205:VAL:O	3:D:206:LYS:CG	2.68	0.41
3:F:160:ASN:HB3	3:F:162:TRP:CZ3	2.55	0.41
1:B:186:LEU:HD22	1:B:199:PHE:CD2	2.55	0.41
2:E:107:TYR:C	2:E:107:TYR:CD1	2.93	0.41
2:E:99:LEU:HD21	2:E:108:PHE:CD2	2.55	0.41
3:F:74:ILE:HG21	3:F:77:MET:HA	2.01	0.41
2:C:2:VAL:HG23	2:C:27:PHE:CE1	2.53	0.41
1:B:241:VAL:O	1:B:241:VAL:HG12	2.20	0.41
2:C:163:ASN:HD21	2:C:201:VAL:HA	1.84	0.41
3:D:136:ASN:HD22	3:D:173:SER:HB3	1.85	0.41
2:E:36:TRP:HA	2:E:96:CYS:HA	2.03	0.41
2:E:144:VAL:O	2:E:144:VAL:CG1	2.68	0.41
1:B:169:LYS:HG2	1:B:170:GLY:H	1.85	0.41
2:C:13:GLN:O	2:C:14:PRO:C	2.58	0.41
2:C:4:LEU:HD12	2:C:4:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:THR:HG22	2:C:91:THR:O	2.19	0.41
2:C:127:PRO:HB3	2:C:153:TYR:CB	2.39	0.41
1:B:212:LEU:CD1	1:B:212:LEU:N	2.76	0.41
1:B:270:ASN:O	1:B:273:VAL:HG12	2.21	0.41
3:F:32:ILE:CG2	3:F:33:HIS:N	2.83	0.41
3:F:51:SER:HB3	3:F:63:GLY:O	2.20	0.41
3:F:202:SER:HA	3:F:203:PRO:HD2	1.84	0.41
2:E:162:TRP:NE1	2:E:171:VAL:HG13	2.34	0.41
1:B:423:LEU:CB	1:B:424:PRO:HD3	2.47	0.41
1:A:309:ALA:O	1:A:311:ALA:N	2.53	0.41
2:E:161:THR:HB	2:E:165:GLY:H	1.85	0.41
1:B:103:GLU:HB3	1:B:111:GLU:HG2	2.02	0.41
2:E:33:TRP:CZ3	2:E:52:ASN:HB3	2.55	0.41
3:D:64:SER:OG	3:D:65:GLY:N	2.53	0.41
1:A:287:ASN:HD22	1:A:290:LYS:CB	2.34	0.41
3:F:29:VAL:O	3:F:67:GLY:HA2	2.21	0.41
1:B:75:TYR:O	1:B:78:LEU:HB3	2.19	0.41
2:C:109:ASP:C	2:C:109:ASP:OD1	2.58	0.41
1:A:219:PHE:O	1:A:220:ILE:C	2.57	0.41
1:B:250:ASN:ND2	2:E:105:TYR:CD1	2.88	0.41
2:C:219:VAL:CB	2:C:220:PRO:HD2	2.51	0.41
2:E:43:LYS:HB3	2:E:43:LYS:HE3	1.86	0.41
1:B:287:ASN:HD21	1:B:289:THR:HB	1.84	0.41
1:B:377:GLU:HG3	1:B:378:LEU:N	2.36	0.41
3:F:197:HIS:C	3:F:197:HIS:ND1	2.74	0.41
1:A:192:ALA:HA	1:A:193:PRO:HD2	1.90	0.41
2:E:125:THR:HA	2:E:126:PRO:HD2	1.83	0.41
2:E:127:PRO:HB2	2:E:150:VAL:CG1	2.50	0.41
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.51	0.41
1:A:305:LEU:HA	1:A:308:VAL:CG2	2.51	0.41
3:D:168:LYS:H	3:D:168:LYS:HG2	1.72	0.41
1:A:341:VAL:O	1:A:345:LEU:HG	2.21	0.41
1:A:218:VAL:O	1:A:221:GLY:N	2.54	0.41
2:E:65:LYS:HB2	2:E:66:ASP:H	1.31	0.41
2:C:165:GLY:O	2:C:167:LEU:N	2.53	0.41
1:B:409:ILE:HD11	1:B:426:ILE:HA	2.03	0.41
3:D:58:PRO:HB3	3:D:60:ARG:NH2	2.36	0.41
2:C:150:VAL:CG2	2:C:205:VAL:CG2	2.99	0.41
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.20	0.41
2:E:87:ARG:CZ	2:E:89:GLU:HB2	2.51	0.41
2:E:18:LEU:CD1	2:E:117:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TRP:CD1	1:A:126:ARG:HG3	2.55	0.41
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.55	0.41
2:E:121:SER:O	2:E:122:ALA:O	2.38	0.41
1:B:109:ILE:N	1:B:110:PRO:CD	2.84	0.41
3:F:138:PHE:HD1	3:F:140:PRO:O	2.05	0.40
3:F:187:ARG:O	3:F:188:HIS:CD2	2.74	0.40
2:C:196:TRP:CD1	2:C:201:VAL:HG23	2.56	0.40
1:B:91:MET:C	1:B:93:GLY:N	2.72	0.40
2:E:167:LEU:HD13	2:E:167:LEU:HA	1.79	0.40
2:C:27:PHE:C	2:C:27:PHE:CD2	2.95	0.40
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.74	0.40
3:D:168:LYS:HB2	3:D:169:ASP:H	1.67	0.40
1:B:65:MET:C	1:B:67:ALA:N	2.75	0.40
1:B:101:ALA:HB3	1:B:130:VAL:HG11	2.02	0.40
2:E:154:PHE:HA	2:E:155:PRO:HA	1.79	0.40
3:D:32:ILE:HA	3:D:32:ILE:HD12	1.81	0.40
1:A:243:LYS:HG3	1:A:243:LYS:O	2.19	0.40
2:E:99:LEU:HD23	2:E:107:TYR:O	2.21	0.40
3:D:201:THR:CG2	3:D:202:SER:H	2.30	0.40
1:A:163:LEU:HD21	1:A:174:ARG:HG3	2.02	0.40
1:B:274:LEU:O	1:B:277:GLN:N	2.50	0.40
1:B:122:VAL:O	1:B:124:TRP:N	2.52	0.40
2:C:76:LYS:O	2:C:77:ASP:C	2.60	0.40
1:A:284:HIS:C	1:A:286:GLY:H	2.25	0.40
1:B:176:THR:HG22	1:B:177:LEU:N	2.36	0.40
1:A:74:ASN:HB3	1:A:77:LEU:HB3	2.04	0.40
2:C:6:GLU:HA	2:C:22:CYS:HA	2.03	0.40
2:E:135:GLY:HA2	3:F:118:PRO:CG	2.51	0.40
1:A:348:PHE:CG	1:A:356:ILE:HB	2.56	0.40
1:A:120:ARG:NH1	1:A:452:THR:HG22	2.37	0.40
1:A:64:ARG:O	1:A:68:LEU:HG	2.20	0.40
2:C:105:TYR:CD2	3:D:30:SER:O	2.73	0.40
2:C:162:TRP:O	2:C:164:SER:N	2.55	0.40
1:A:358:ALA:N	1:A:359:PRO:CD	2.84	0.40
1:A:42:VAL:CG2	1:A:159:GLY:HA2	2.52	0.40
1:A:114:GLY:HA2	1:A:449:LEU:HD21	2.02	0.40
1:B:135:GLY:HA2	1:B:138:THR:OG1	2.22	0.40
1:A:270:ASN:CA	1:A:273:VAL:HG12	2.52	0.40
1:A:356:ILE:O	1:A:360:MET:HE3	2.21	0.40
2:C:217:LYS:O	2:C:219:VAL:HG13	2.22	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%)	361 (82%)	62 (14%)	19 (4%)	3	25
1	B	439/473 (93%)	342 (78%)	81 (18%)	16 (4%)	4	30
2	C	219/222 (99%)	166 (76%)	39 (18%)	14 (6%)	2	13
2	E	219/222 (99%)	173 (79%)	30 (14%)	16 (7%)	1	9
3	D	209/211 (99%)	159 (76%)	28 (13%)	22 (10%)	1	4
3	F	209/211 (99%)	158 (76%)	33 (16%)	18 (9%)	1	6
All	All	1737/1812 (96%)	1359 (78%)	273 (16%)	105 (6%)	2	16

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	209	ARG
1	A	236	VAL
1	A	309	ALA
1	B	73	ASP
1	B	132	PHE
2	C	27	PHE
2	C	65	LYS
2	C	140	ALA
3	D	7	SER
3	D	67	GLY
3	D	126	SER
3	D	137	ASN
3	D	168	LYS
3	D	169	ASP
2	E	51	ILE
2	E	65	LYS
2	E	113	ALA
2	E	122	ALA
2	E	140	ALA

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Mol	Chain	Res	Type
3	F	2	ILE
3	F	7	SER
3	F	109	ASP
3	F	111	ALA
3	F	139	TYR
3	F	140	PRO
3	F	153	GLU
1	A	283	VAL
1	A	419	TYR
1	B	209	ARG
1	B	283	VAL
1	B	309	ALA
1	B	441	GLY
1	B	444	LEU
2	C	164	SER
2	C	166	SER
2	C	196	TRP
3	D	31	TYR
3	D	55	SER
3	D	109	ASP
3	D	127	GLY
3	D	139	TYR
3	D	153	GLU
3	D	198	LYS
2	E	138	ALA
2	E	180	ALA
3	F	66	SER
3	F	67	GLY
3	F	119	PRO
3	F	125	THR
3	F	184	GLU
1	A	102	PRO
1	A	132	PHE
1	A	149	GLY
1	A	413	LEU
1	A	444	LEU
1	B	102	PRO
1	B	310	PRO
2	C	18	LEU
2	C	138	ALA
2	C	220	PRO
3	D	46	TRP

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Mol	Chain	Res	Type
3	D	50	THR
3	D	90	TRP
2	E	62	PRO
3	F	137	ASN
3	F	203	PRO
1	A	250	ASN
1	A	310	PRO
1	B	95	PHE
1	B	188	ALA
2	C	31	ARG
2	C	163	ASN
3	D	23	CYS
3	D	59	VAL
3	D	141	LYS
3	D	152	SER
3	F	50	THR
3	F	79	ALA
3	F	112	PRO
1	A	206	PRO
1	B	206	PRO
1	B	443	PRO
3	D	187	ARG
2	E	52	ASN
2	E	157	PRO
2	E	165	GLY
2	E	211	SER
3	F	165	GLN
1	B	123	ARG
1	B	235	GLU
2	C	53	PRO
2	C	197	PRO
3	D	80	GLU
2	E	196	TRP
1	A	201	ILE
2	E	37	VAL
2	E	53	PRO
2	C	174	PHE
2	E	69	ILE
1	A	261	ILE
1	B	149	GLY
1	A	101	ALA
1	A	443	PRO

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Mol	Chain	Res	Type
1	A	285	GLY

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%)	312 (93%)	23 (7%)	19	59
1	B	332/358 (93%)	310 (93%)	22 (7%)	21	61
2	C	181/182 (100%)	149 (82%)	32 (18%)	2	11
2	E	181/182 (100%)	141 (78%)	40 (22%)	1	5
3	D	185/185 (100%)	153 (83%)	32 (17%)	2	12
3	F	185/185 (100%)	156 (84%)	29 (16%)	3	15
All	All	1399/1450 (96%)	1221 (87%)	178 (13%)	5	25

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	69	VAL
1	A	70	HIS
1	A	73	ASP
1	A	74	ASN
1	A	103	GLU
1	A	111	GLU
1	A	148	GLU
1	A	176	THR
1	A	200	ILE
1	A	205	ARG
1	A	208	PHE
1	A	209	ARG
1	A	211	THR
1	A	212	LEU
1	A	277	GLN
1	A	324	THR

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Mol	Chain	Res	Type
1	A	381	GLN
1	A	397	LEU
1	A	402	ILE
1	A	420	GLN
1	A	445	TYR
1	A	451	ARG
1	B	65	MET
1	B	70	HIS
1	B	73	ASP
1	B	74	ASN
1	B	103	GLU
1	B	111	GLU
1	B	148	GLU
1	B	150	PRO
1	B	176	THR
1	B	177	LEU
1	B	180	THR
1	B	205	ARG
1	B	208	PHE
1	B	212	LEU
1	B	277	GLN
1	B	324	THR
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	445	TYR
1	B	451	ARG
2	C	3	ARG
2	C	4	LEU
2	C	5	LEU
2	C	6	GLU
2	C	13	GLN
2	C	41	PRO
2	C	45	LEU
2	C	51	ILE
2	C	53	PRO
2	C	55	SER
2	C	67	LYS
2	C	72	ARG
2	C	87	ARG
2	C	98	ARG

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Mol	Chain	Res	Type
2	C	110	VAL
2	C	128	SER
2	C	136	SER
2	C	151	LYS
2	C	155	PRO
2	C	157	PRO
2	C	158	VAL
2	C	167	LEU
2	C	174	PHE
2	C	185	LEU
2	C	200	THR
2	C	202	THR
2	C	203	CYS
2	C	204	ASN
2	C	211	SER
2	C	212	THR
2	C	219	VAL
2	C	221	ARG
3	D	1	ASP
3	D	6	GLN
3	D	20	THR
3	D	24	SER
3	D	32	ILE
3	D	41	THR
3	D	44	LYS
3	D	46	TRP
3	D	50	THR
3	D	59	VAL
3	D	64	SER
3	D	68	THR
3	D	72	LEU
3	D	77	MET
3	D	94	PRO
3	D	95	GLN
3	D	115	SER
3	D	117	PHE
3	D	120	SER
3	D	122	GLU
3	D	125	THR
3	D	137	ASN
3	D	156	ASN
3	D	159	LEU

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Mol	Chain	Res	Type
3	D	163	THR
3	D	175	SER
3	D	181	THR
3	D	183	ASP
3	D	192	THR
3	D	202	SER
3	D	205	VAL
3	D	206	LYS
2	E	2	VAL
2	E	4	LEU
2	E	5	LEU
2	E	6	GLU
2	E	12	VAL
2	E	18	LEU
2	E	22	CYS
2	E	27	PHE
2	E	30	SER
2	E	45	LEU
2	E	48	ILE
2	E	51	ILE
2	E	53	PRO
2	E	54	VAL
2	E	55	SER
2	E	58	ILE
2	E	59	ASN
2	E	61	THR
2	E	62	PRO
2	E	67	LYS
2	E	72	ARG
2	E	77	ASP
2	E	83	ILE
2	E	107	TYR
2	E	118	THR
2	E	121	SER
2	E	125	THR
2	E	146	LEU
2	E	151	LYS
2	E	167	LEU
2	E	172	HIS
2	E	177	VAL
2	E	179	GLN
2	E	185	LEU

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Mol	Chain	Res	Type
2	E	187	SER
2	E	188	SER
2	E	193	SER
2	E	200	THR
2	E	203	CYS
2	E	204	ASN
3	F	1	ASP
3	F	5	THR
3	F	6	GLN
3	F	17	ASP
3	F	28	SER
3	F	30	SER
3	F	42	SER
3	F	44	LYS
3	F	48	TYR
3	F	54	THR
3	F	88	GLN
3	F	91	SER
3	F	116	ILE
3	F	119	PRO
3	F	121	SER
3	F	143	ILE
3	F	153	GLU
3	F	158	VAL
3	F	162	TRP
3	F	166	ASP
3	F	175	SER
3	F	179	THR
3	F	181	THR
3	F	187	ARG
3	F	189	ASN
3	F	194	GLU
3	F	201	THR
3	F	208	PHE
3	F	210	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	153	GLN
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	207	GLN
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	420	GLN
1	A	437	GLN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	207	GLN
1	B	270	ASN
1	B	277	GLN
1	B	284	HIS
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	437	GLN
2	C	39	GLN
2	C	172	HIS
3	D	37	GLN
3	D	93	HIS
3	D	136	ASN
3	D	137	ASN
3	D	155	GLN
3	D	189	ASN
2	E	39	GLN
3	F	37	GLN
3	F	89	GLN
3	F	137	ASN
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 ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/473 (93%)	-0.36	2 (0%) 91 87	48, 77, 111, 138	0
1	B	441/473 (93%)	-0.43	1 (0%) 95 94	41, 71, 115, 151	0
2	C	221/222 (99%)	-0.24	2 (0%) 85 78	43, 71, 106, 160	0
2	E	221/222 (99%)	-0.05	3 (1%) 78 65	37, 78, 121, 145	0
3	D	211/211 (100%)	-0.00	1 (0%) 91 87	52, 91, 118, 128	0
3	F	211/211 (100%)	-0.10	3 (1%) 78 65	26, 70, 123, 140	0
All	All	1749/1812 (96%)	-0.25	12 (0%) 89 83	26, 76, 117, 160	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	222	ALA	3.8
1	B	235	GLU	3.6
1	A	235	GLU	2.8
1	A	72	ALA	2.8
2	C	136	SER	2.4
3	F	156	ASN	2.2
2	C	139	ALA	2.2
3	F	153	GLU	2.2
2	E	35	SER	2.2
2	E	42	GLY	2.2
3	D	40	GLY	2.1
3	F	155	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.