



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:38 PM GMT

PDB ID : 1UIJ
Title : Crystal Structure Of Soybean beta-Conglycinin Beta Homotrimer (I122M/K124W)
Authors : Maruyama, N.; Maruyama, Y.; Tsuruki, T.; Okuda, E.; Yoshikawa, M.; Utsumi, S.
Deposited on : 2003-07-16
Resolution : 2.50 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

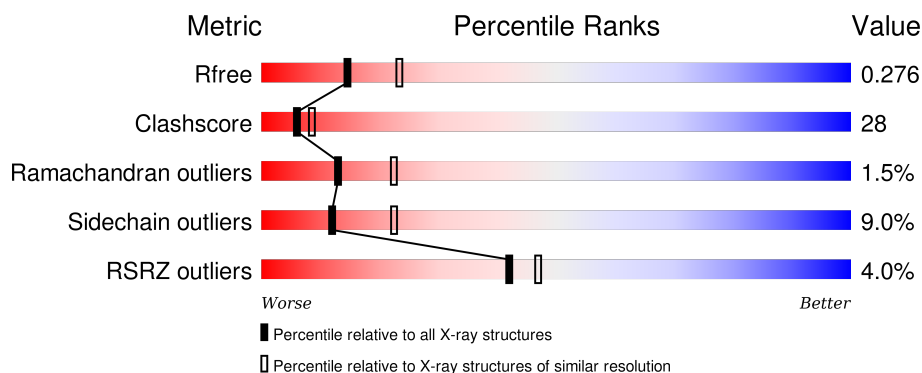
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	416	<div> <div>2%</div> <div>52% 33% 5% 9%</div> </div>
1	B	416	<div> <div>3%</div> <div>47% 36% 5% 11%</div> </div>
1	C	416	<div> <div>6%</div> <div>40% 38% 5% 17%</div> </div>
1	D	416	<div> <div>2%</div> <div>49% 36% 6% 9%</div> </div>
1	E	416	<div> <div>3%</div> <div>46% 39% • 11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	416	<div><div></div><div>5%</div><div>37%</div><div>41%</div><div>5%</div><div>17%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18133 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 beta subunit of beta conglycinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3087	1947	550	589	1			
1	B	370	Total	C	N	O	S	0	0	0
			3022	1911	538	572	1			
1	C	346	Total	C	N	O	S	0	0	0
			2824	1797	494	532	1			
1	D	377	Total	C	N	O	S	0	0	0
			3087	1947	550	589	1			
1	E	370	Total	C	N	O	S	0	0	0
			3022	1911	538	572	1			
1	F	346	Total	C	N	O	S	0	0	0
			2824	1797	494	532	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	MET	ILE	ENGINEERED	UNP P25974
A	124	TRP	LYS	ENGINEERED	UNP P25974
B	122	MET	ILE	ENGINEERED	UNP P25974
B	124	TRP	LYS	ENGINEERED	UNP P25974
C	122	MET	ILE	ENGINEERED	UNP P25974
C	124	TRP	LYS	ENGINEERED	UNP P25974
D	122	MET	ILE	ENGINEERED	UNP P25974
D	124	TRP	LYS	ENGINEERED	UNP P25974
E	122	MET	ILE	ENGINEERED	UNP P25974
E	124	TRP	LYS	ENGINEERED	UNP P25974
F	122	MET	ILE	ENGINEERED	UNP P25974
F	124	TRP	LYS	ENGINEERED	UNP P25974

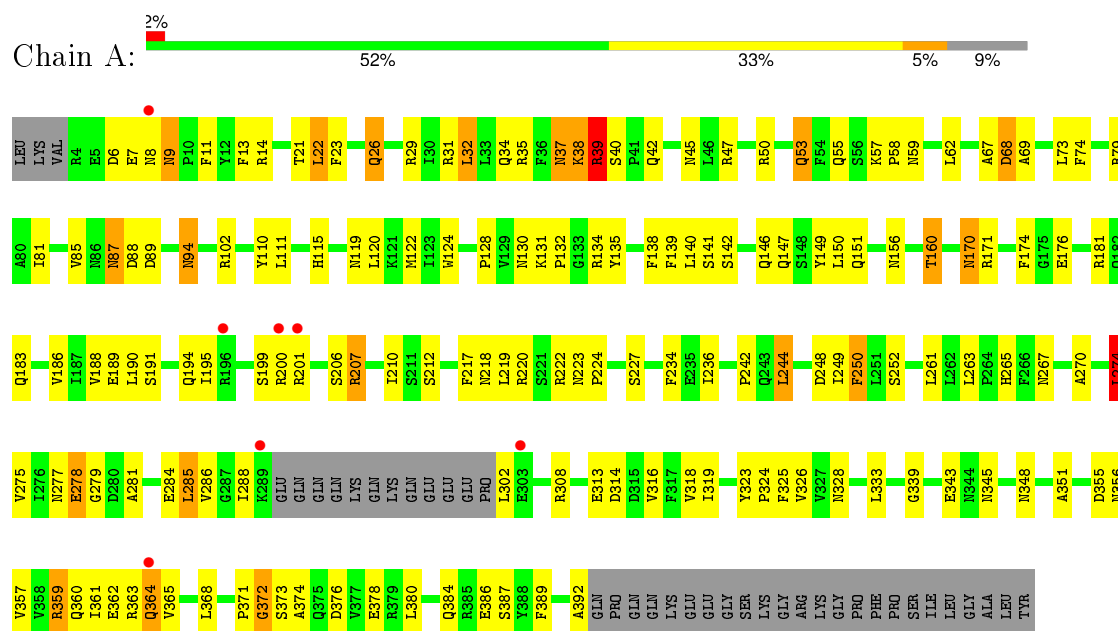
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total 62	O 62	0	0
2	B	53	Total 53	O 53	0	0
2	C	19	Total 19	O 19	0	0
2	D	65	Total 65	O 65	0	0
2	E	47	Total 47	O 47	0	0
2	F	21	Total 21	O 21	0	0

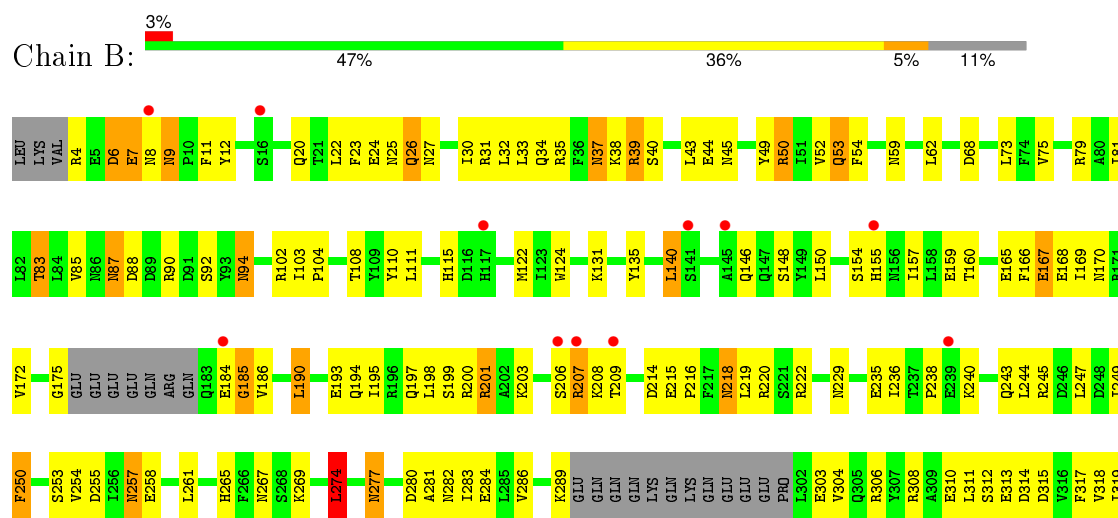
3 Residue-property plots

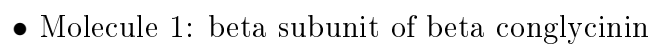
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



- Molecule 1: beta subunit of beta conglycinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.26Å 62.58Å 159.01Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 93.8 (20.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.273 0.225 , 0.276	Depositor DCC
R_{free} test set	4153 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.4	EDS
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 84125 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18133	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/3150	0.68	1/4260 (0.0%)
1	B	0.40	0/3084	0.67	1/4171 (0.0%)
1	C	0.34	0/2886	0.61	0/3910
1	D	0.39	0/3150	0.68	1/4260 (0.0%)
1	E	0.39	0/3084	0.65	0/4171
1	F	0.35	0/2886	0.62	1/3910 (0.0%)
All	All	0.38	0/18240	0.66	4/24682 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	LEU	CA-CB-CG	6.46	130.16	115.30
1	F	251	LEU	CA-CB-CG	5.72	128.46	115.30
1	D	274	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	274	LEU	CA-CB-CG	5.34	127.59	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3087	0	3004	150	0
1	B	3022	0	2950	157	0
1	C	2824	0	2739	202	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3087	0	3004	163	0
1	E	3022	0	2950	176	0
1	F	2824	0	2739	210	0
2	A	62	0	0	3	0
2	B	53	0	0	3	0
2	C	19	0	0	0	0
2	D	65	0	0	4	0
2	E	47	0	0	5	0
2	F	21	0	0	2	0
All	All	18133	0	17386	1002	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 28.

All (1002) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASN:HD22	1:B:195:ILE:HD12	1.03	1.07
1:E:90:ARG:HH11	1:F:362:GLU:HG2	1.19	1.05
1:E:59:ASN:HD22	1:E:195:ILE:HD12	1.20	1.05
1:A:26:GLN:HE21	1:A:26:GLN:H	1.04	1.03
1:A:183:GLN:HG2	1:A:188:VAL:HG11	1.42	1.01
1:B:26:GLN:H	1:B:26:GLN:NE2	1.61	0.99
1:E:37:ASN:HD22	1:E:37:ASN:H	1.11	0.98
1:E:90:ARG:NH1	1:F:362:GLU:HG2	1.79	0.98
1:B:111:LEU:HD21	1:B:122:MET:HE1	1.46	0.97
1:E:79:ARG:HD2	1:E:94:ASN:HD21	1.29	0.96
1:D:183:GLN:HG2	1:D:188:VAL:HG11	1.45	0.96
1:A:348:ASN:HD22	1:A:357:VAL:HB	1.29	0.95
1:C:384:GLN:HE21	1:C:386:GLU:H	1.08	0.94
1:C:384:GLN:NE2	1:C:386:GLU:HB2	1.83	0.93
1:E:111:LEU:HD21	1:E:122:MET:HE2	1.49	0.92
1:A:111:LEU:HD21	1:A:122:MET:HE3	1.51	0.92
1:B:111:LEU:HD21	1:B:122:MET:CE	2.00	0.91
1:B:59:ASN:HD22	1:B:195:ILE:CD1	1.82	0.91
1:A:261:LEU:HD22	1:A:392:ALA:HB2	1.52	0.91
1:B:261:LEU:HD22	1:B:392:ALA:HB2	1.51	0.90
1:B:59:ASN:ND2	1:B:195:ILE:HD12	1.86	0.90
1:C:50:ARG:HH21	1:C:50:ARG:HB3	1.35	0.90
1:A:37:ASN:H	1:A:37:ASN:HD22	1.20	0.90
1:B:79:ARG:NH1	1:B:94:ASN:HD21	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLN:NE2	1:A:364:GLN:H	1.71	0.88
1:D:29:ARG:HD3	1:D:31:ARG:HG3	1.56	0.87
1:B:26:GLN:H	1:B:26:GLN:HE21	1.22	0.87
1:F:79:ARG:HE	1:F:94:ASN:HD21	1.20	0.86
1:B:37:ASN:H	1:B:37:ASN:HD22	1.19	0.86
1:E:218:ASN:HD22	1:E:220:ARG:H	1.23	0.86
1:D:111:LEU:HD21	1:D:122:MET:HE2	1.56	0.85
1:A:35:ARG:NH1	1:A:134:ARG:HD2	1.92	0.84
1:C:170:ASN:HD22	1:C:174:PHE:HB2	1.43	0.83
1:A:371:PRO:HG3	1:C:174:PHE:O	1.78	0.83
1:E:111:LEU:HD21	1:E:122:MET:CE	2.08	0.82
1:C:13:PHE:CE1	1:C:39:ARG:HG3	2.14	0.82
1:F:14:ARG:HG2	1:F:16:SER:HB3	1.61	0.82
1:D:111:LEU:HD21	1:D:122:MET:CE	2.10	0.82
1:F:34:GLN:NE2	1:F:39:ARG:HG2	1.93	0.82
1:C:32:LEU:HD23	1:C:52:VAL:HG22	1.60	0.82
1:F:302:LEU:H	1:F:302:LEU:HD22	1.43	0.81
1:A:218:ASN:ND2	1:A:220:ARG:H	1.77	0.81
1:E:207:ARG:HH11	1:E:207:ARG:HB3	1.44	0.81
1:D:218:ASN:HD22	1:D:220:ARG:H	1.26	0.81
1:D:176:GLU:HB2	2:D:437:HOH:O	1.79	0.81
1:A:26:GLN:HE21	1:A:26:GLN:N	1.78	0.81
1:A:26:GLN:NE2	1:A:26:GLN:H	1.78	0.81
1:D:34:GLN:OE1	1:D:39:ARG:HD2	1.80	0.80
1:C:386:GLU:HB3	1:C:390:VAL:HG12	1.62	0.80
1:B:79:ARG:HH11	1:B:94:ASN:HD21	1.24	0.80
1:A:156:ASN:O	1:A:160:THR:HG22	1.80	0.80
1:C:170:ASN:ND2	1:C:174:PHE:HB2	1.95	0.79
1:B:219:LEU:HD13	1:B:236:ILE:HG12	1.65	0.79
1:C:79:ARG:HD2	1:C:94:ASN:HD21	1.48	0.78
1:E:26:GLN:H	1:E:26:GLN:NE2	1.82	0.78
1:F:111:LEU:HD21	1:F:122:MET:CE	2.14	0.77
1:C:214:THR:H	1:C:217:LYS:HE3	1.49	0.77
1:A:218:ASN:HD22	1:A:220:ARG:H	1.31	0.77
1:A:355:ASP:HA	1:C:87:ASN:O	1.84	0.77
1:E:59:ASN:HA	1:E:195:ILE:HD11	1.66	0.76
1:A:189:GLU:O	1:A:190:LEU:HD12	1.84	0.76
1:B:44:GLU:HG3	2:B:435:HOH:O	1.84	0.76
1:F:52:VAL:HB	1:F:124:TRP:HB2	1.67	0.76
1:D:261:LEU:HD21	1:D:390:VAL:HG22	1.68	0.75
1:A:111:LEU:HD21	1:A:122:MET:CE	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:LEU:HD21	1:D:390:VAL:CG2	2.16	0.75
1:A:29:ARG:HD3	1:A:31:ARG:HG3	1.67	0.75
1:C:236:GLY:O	1:C:392:ALA:HB3	1.87	0.75
1:A:384:GLN:HE21	1:A:386:GLU:H	1.33	0.75
1:F:196:LEU:HD13	1:F:213:ILE:HG12	1.67	0.75
1:A:261:LEU:HB3	1:A:328:ASN:HD22	1.52	0.75
1:E:37:ASN:HD22	1:E:37:ASN:N	1.85	0.75
1:C:35:ARG:HG2	1:C:50:ARG:HE	1.51	0.75
1:D:218:ASN:ND2	1:D:220:ARG:H	1.85	0.74
1:B:81:ILE:CD1	1:B:199:SER:HB3	2.17	0.74
1:F:15:SER:HB3	1:F:314:ASP:O	1.87	0.74
1:A:38:LYS:HD3	1:A:39:ARG:N	2.02	0.74
1:D:191:SER:OG	1:D:194:GLN:HG3	1.86	0.74
1:B:32:LEU:HD11	1:B:50:ARG:CZ	2.16	0.74
1:E:277:ASN:HB3	1:E:334:ASN:HD22	1.52	0.74
1:C:6:ASP:O	1:C:8:ASN:N	2.20	0.74
1:A:81:ILE:HD13	1:A:199:SER:HA	1.68	0.74
1:F:31:ARG:HE	1:F:53:GLN:HE21	1.33	0.73
1:A:380:LEU:HD11	1:C:169:ILE:HA	1.69	0.73
1:F:111:LEU:HD21	1:F:122:MET:HE1	1.71	0.73
1:C:306:ARG:HD3	1:C:308:ARG:NH1	2.02	0.73
1:D:17:ASN:C	1:D:17:ASN:HD22	1.91	0.73
1:E:59:ASN:HA	1:E:195:ILE:CD1	2.17	0.73
1:C:199:ARG:HD3	1:C:213:ILE:CD1	2.19	0.73
1:F:13:PHE:CE1	1:F:39:ARG:HG3	2.24	0.72
1:B:140:LEU:HD11	1:C:358:VAL:HG22	1.71	0.72
1:C:30:ILE:HG12	1:C:54:PHE:HD1	1.54	0.72
1:C:214:THR:H	1:C:217:LYS:CE	2.02	0.72
1:D:207:ARG:HH11	1:D:207:ARG:HG3	1.55	0.71
1:A:356:ASN:HB3	1:A:359:ARG:HG2	1.72	0.71
1:F:384:GLN:HE21	1:F:386:GLU:H	1.37	0.71
1:E:110:TYR:OH	1:F:362:GLU:HG3	1.90	0.71
1:E:169:ILE:HA	1:F:380:LEU:HD11	1.73	0.71
1:C:306:ARG:HD3	1:C:308:ARG:HH12	1.56	0.71
1:B:382:LYS:HZ3	1:B:385:ARG:HH12	1.38	0.71
1:E:363:ARG:HG2	1:E:378:GLU:OE1	1.90	0.70
1:D:363:ARG:HG2	1:D:374:ALA:HB1	1.72	0.70
1:B:363:ARG:HG2	1:B:378:GLU:OE1	1.91	0.70
1:E:218:ASN:ND2	1:E:220:ARG:H	1.90	0.70
1:A:261:LEU:HB3	1:A:328:ASN:ND2	2.05	0.70
1:E:102:ARG:HB3	1:E:243:GLN:HE21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:N	1:B:257:ASN:HD22	1.89	0.69
1:E:59:ASN:ND2	1:E:195:ILE:HD12	2.01	0.69
1:C:102:ARG:H	1:C:220:GLN:NE2	1.90	0.69
1:B:39:ARG:HG3	1:B:40:SER:N	2.07	0.69
1:D:306:ARG:HD2	1:D:308:ARG:NH2	2.07	0.69
1:D:384:GLN:HE21	1:D:386:GLU:H	1.39	0.69
1:A:59:ASN:HA	1:A:195:ILE:HD11	1.74	0.69
1:B:90:ARG:CZ	1:C:362:GLU:HG2	2.22	0.69
1:F:205:ASN:HD21	1:F:389:PHE:HB2	1.58	0.69
1:A:68:ASP:HB3	1:A:135:TYR:HB2	1.75	0.69
1:C:35:ARG:CG	1:C:50:ARG:HE	2.06	0.69
1:D:37:ASN:HD22	1:D:37:ASN:H	1.41	0.69
1:D:198:LEU:HD21	1:E:364:GLN:HB2	1.75	0.68
1:A:87:ASN:HD22	1:A:88:ASP:N	1.91	0.68
1:C:254:ASN:HB3	1:C:334:ASN:HD22	1.59	0.68
1:F:235:GLU:H	1:F:332:ASN:HD22	1.40	0.68
1:B:219:LEU:CD1	1:B:236:ILE:HG12	2.22	0.68
1:E:32:LEU:HD11	1:E:50:ARG:CZ	2.23	0.68
1:D:258:GLU:HG3	1:D:331:SER:HA	1.76	0.68
1:B:377:VAL:O	1:B:381:LEU:HG	1.92	0.68
1:C:260:ILE:HD12	1:C:311:LEU:HD11	1.76	0.68
1:A:35:ARG:HH12	1:A:134:ARG:HD2	1.59	0.68
1:A:35:ARG:HG3	1:A:50:ARG:NH2	2.09	0.68
1:E:207:ARG:CB	1:E:207:ARG:HH11	2.07	0.68
1:D:210:ILE:HD11	1:D:236:ILE:HD12	1.76	0.68
1:F:233:ILE:HD12	1:F:333:LEU:HD23	1.74	0.67
1:B:160:THR:HG21	1:C:392:ALA:HB2	1.76	0.67
1:D:357:VAL:HG23	1:F:86:ASN:O	1.95	0.67
1:F:221:LEU:HG	1:F:226:ILE:O	1.94	0.67
1:A:368:LEU:HD23	1:C:188:VAL:HG21	1.77	0.67
1:E:61:ILE:HB	1:E:112:VAL:HG22	1.77	0.67
1:E:4:ARG:HB2	1:E:306:ARG:O	1.95	0.66
1:D:59:ASN:HA	1:D:195:ILE:HD11	1.77	0.66
1:C:13:PHE:HE1	1:C:39:ARG:HG3	1.60	0.66
1:F:37:ASN:H	1:F:37:ASN:HD22	1.40	0.66
1:D:85:VAL:HG23	1:E:360:GLN:HB2	1.77	0.66
1:A:69:ALA:HB2	1:A:128:PRO:HA	1.78	0.66
1:D:238:PRO:HB3	1:D:245:ARG:HA	1.78	0.66
1:C:39:ARG:HG2	1:C:39:ARG:HH11	1.59	0.66
1:C:14:ARG:HG2	1:C:16:SER:HB3	1.78	0.66
1:D:29:ARG:HD3	1:D:31:ARG:CG	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ASN:HD22	1:D:9:ASN:C	1.99	0.66
1:D:183:GLN:CG	1:D:188:VAL:HG11	2.22	0.65
1:E:81:ILE:HD13	1:E:199:SER:HA	1.78	0.65
1:B:155:HIS:O	1:B:159:GLU:HG3	1.96	0.65
1:B:283:ILE:HD12	1:B:311:LEU:HD11	1.78	0.65
1:A:34:GLN:NE2	1:A:38:LYS:HE2	2.12	0.65
1:F:313:GLU:O	1:F:314:ASP:HB2	1.96	0.65
1:F:132:PRO:HA	2:F:421:HOH:O	1.95	0.65
1:A:35:ARG:CG	1:A:50:ARG:NH2	2.59	0.65
1:B:6:ASP:O	1:B:7:GLU:HB2	1.97	0.65
1:B:37:ASN:N	1:B:37:ASN:HD22	1.90	0.65
1:F:37:ASN:HD22	1:F:37:ASN:N	1.93	0.65
1:F:260:ILE:HD12	1:F:311:LEU:HD11	1.79	0.65
1:B:284:GLU:HG2	1:B:308:ARG:HG2	1.77	0.65
1:F:234:ASN:HD22	1:F:234:ASN:N	1.95	0.65
1:C:151:GLN:HG2	1:C:174:PHE:CZ	2.31	0.65
1:C:199:ARG:HD3	1:C:213:ILE:HD11	1.79	0.64
1:D:59:ASN:HD22	1:D:195:ILE:CD1	2.10	0.64
1:D:156:ASN:O	1:D:160:THR:HG22	1.97	0.64
1:C:379:ARG:HG3	1:C:379:ARG:HH11	1.62	0.64
1:E:384:GLN:HE21	1:E:386:GLU:H	1.45	0.64
1:F:258:ALA:HB2	1:F:333:LEU:HD22	1.80	0.64
1:F:197:ARG:HH22	1:F:232:ASP:CG	2.01	0.64
1:C:239:LEU:O	1:C:326:VAL:HG23	1.97	0.64
1:F:261:GLU:CD	1:F:308:ARG:HH21	2.01	0.64
1:A:183:GLN:HG2	1:A:188:VAL:CG1	2.25	0.63
1:D:358:VAL:HG22	1:F:140:LEU:HD11	1.79	0.63
1:D:35:ARG:HB2	1:D:38:LYS:HB3	1.81	0.63
1:D:237:THR:H	1:D:240:LYS:HE3	1.64	0.63
1:C:373:SER:O	1:C:377:VAL:HG23	1.98	0.63
1:A:183:GLN:CG	1:A:188:VAL:HG11	2.24	0.63
1:F:199:ARG:HH12	1:F:217:LYS:HD2	1.62	0.63
1:C:252:VAL:HG22	1:C:336:LEU:HB3	1.81	0.63
1:C:378:GLU:O	1:C:382:LYS:HG3	1.99	0.63
1:C:195:ASN:HB3	1:C:198:SER:HB2	1.80	0.63
1:C:50:ARG:HH21	1:C:50:ARG:CB	2.11	0.63
1:B:81:ILE:HD13	1:B:199:SER:HB3	1.79	0.63
1:E:168:GLU:O	1:E:172:VAL:HG23	1.99	0.63
1:E:218:ASN:HD21	1:E:220:ARG:HB2	1.63	0.63
1:F:195:ASN:HD22	1:F:198:SER:N	1.96	0.63
1:E:122:MET:CE	1:E:124:TRP:HE1	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ASN:ND2	1:F:174:PHE:HB2	2.13	0.62
1:D:59:ASN:ND2	1:D:195:ILE:HD12	2.14	0.62
1:F:364:GLN:H	1:F:364:GLN:CD	2.03	0.62
1:D:189:GLU:O	1:D:190:LEU:HD23	1.99	0.62
1:E:83:THR:HB	1:E:92:SER:OG	2.00	0.62
1:B:73:LEU:HG	1:B:124:TRP:CD1	2.35	0.62
1:C:214:THR:OG1	1:C:217:LYS:HE2	2.00	0.62
1:D:285:LEU:HD21	1:D:323:TYR:HB3	1.79	0.62
1:E:116:ASP:CG	1:E:192:LYS:HE3	2.20	0.62
1:B:258:GLU:H	1:B:332:ASN:HD22	1.47	0.62
1:B:277:ASN:HB3	1:B:334:ASN:HD22	1.64	0.61
1:B:269:LYS:H	1:B:345:ASN:HD22	1.47	0.61
1:E:87:ASN:HD22	1:E:88:ASP:N	1.97	0.61
1:C:151:GLN:HG2	1:C:174:PHE:CE1	2.35	0.61
1:F:238:LEU:HD22	1:F:392:ALA:HB2	1.81	0.61
1:A:212:SER:O	1:A:242:PRO:HG2	2.00	0.61
1:E:206:SER:H	1:E:209:THR:CG2	2.13	0.61
1:B:382:LYS:HE2	1:B:385:ARG:NH2	2.15	0.61
1:D:355:ASP:HA	1:F:87:ASN:O	2.01	0.61
1:C:80:ALA:HB2	1:C:120:LEU:HD13	1.83	0.61
1:F:235:GLU:H	1:F:332:ASN:ND2	1.97	0.61
1:D:252:SER:OG	1:D:337:ALA:HB3	2.00	0.61
1:F:306:ARG:HD3	1:F:308:ARG:HH12	1.66	0.61
1:E:37:ASN:H	1:E:37:ASN:ND2	1.91	0.61
1:F:39:ARG:HH11	1:F:39:ARG:HG2	1.66	0.61
1:D:261:LEU:HD23	1:D:261:LEU:H	1.66	0.60
1:D:349:PHE:O	1:D:356:ASN:HA	2.02	0.60
1:D:31:ARG:HH21	1:D:53:GLN:NE2	1.98	0.60
1:A:35:ARG:N	1:A:50:ARG:NH2	2.48	0.60
1:A:263:LEU:HD13	1:A:351:ALA:O	2.00	0.60
1:E:79:ARG:HD2	1:E:94:ASN:ND2	2.09	0.60
1:C:384:GLN:HE21	1:C:386:GLU:N	1.90	0.60
1:A:131:LYS:HE2	2:A:442:HOH:O	2.01	0.60
1:C:252:VAL:CG2	1:C:336:LEU:HB3	2.32	0.60
1:E:31:ARG:HH21	1:E:53:GLN:HE22	1.49	0.60
1:C:207:PHE:CE1	1:C:391:ASP:HB2	2.36	0.60
1:B:261:LEU:N	1:B:261:LEU:HD23	2.17	0.60
1:C:312:SER:O	1:C:315:ASP:HB2	2.01	0.60
1:A:170:ASN:HD22	1:A:174:PHE:HB2	1.67	0.60
1:B:26:GLN:HE21	1:B:26:GLN:N	1.97	0.60
1:C:262:LEU:HD21	1:C:323:TYR:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:LEU:HD12	1:F:388:TYR:N	2.16	0.60
1:B:87:ASN:HD22	1:B:88:ASP:N	1.98	0.60
1:F:31:ARG:HE	1:F:53:GLN:NE2	1.98	0.60
1:A:274:LEU:HD12	1:A:274:LEU:C	2.22	0.60
1:E:172:VAL:HG11	1:F:376:ASP:O	2.01	0.60
1:F:359:ARG:HD3	1:F:381:LEU:O	2.02	0.60
1:F:79:ARG:O	1:F:120:LEU:HD13	2.02	0.59
1:E:102:ARG:H	1:E:243:GLN:NE2	2.00	0.59
1:D:222:ARG:HG3	1:D:222:ARG:HH21	1.67	0.59
1:C:246:LYS:H	1:C:345:ASN:ND2	2.01	0.59
1:C:61:ILE:CD1	1:C:112:VAL:HG22	2.33	0.59
1:F:9:ASN:C	1:F:9:ASN:HD22	2.04	0.59
1:B:289:LYS:N	1:B:303:GLU:O	2.34	0.59
1:F:170:ASN:HD22	1:F:174:PHE:HB2	1.67	0.59
1:A:37:ASN:N	1:A:37:ASN:HD22	1.92	0.59
1:A:34:GLN:CD	1:A:38:LYS:HE2	2.22	0.59
1:E:313:GLU:O	1:E:314:ASP:HB2	2.03	0.59
1:D:116:ASP:OD1	1:D:192:LYS:HE2	2.03	0.59
1:F:111:LEU:HD21	1:F:122:MET:HE2	1.85	0.59
1:C:227:PHE:C	1:C:227:PHE:CD2	2.76	0.59
1:C:251:LEU:C	1:C:251:LEU:HD12	2.23	0.59
1:C:196:LEU:HD23	1:C:230:SER:HB2	1.85	0.59
1:D:87:ASN:HD22	1:D:88:ASP:N	2.00	0.59
1:F:102:ARG:HB3	1:F:220:GLN:HE21	1.68	0.59
1:C:32:LEU:HD13	1:C:50:ARG:HH22	1.67	0.58
1:C:263:VAL:CG1	1:C:324:PRO:HB2	2.33	0.58
1:D:218:ASN:HD22	1:D:220:ARG:N	1.99	0.58
1:C:61:ILE:HD12	1:C:112:VAL:HG22	1.85	0.58
1:D:68:ASP:HB3	1:D:135:TYR:HB2	1.83	0.58
1:D:363:ARG:CG	1:D:374:ALA:HB1	2.33	0.58
1:F:244:ASN:HB3	1:F:345:ASN:HD21	1.68	0.58
1:E:353:GLU:OE1	1:E:385:ARG:NH1	2.37	0.58
1:C:119:ASN:HD22	1:C:119:ASN:N	2.02	0.58
1:F:57:LYS:HB3	1:F:58:PRO:HD2	1.86	0.58
1:A:191:SER:OG	1:A:194:GLN:HG3	2.03	0.58
1:B:218:ASN:ND2	1:B:220:ARG:H	2.02	0.58
1:B:35:ARG:HD2	1:B:38:LYS:HD2	1.85	0.58
1:B:200:ARG:HG3	1:B:201:ARG:HG3	1.85	0.58
1:F:330:THR:O	1:F:331:SER:HB3	2.03	0.58
1:A:210:ILE:HD11	1:A:236:ILE:HD12	1.86	0.58
1:F:253:ILE:HD11	1:F:311:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:NH1	1:D:134:ARG:HD2	2.19	0.58
1:D:288:ILE:HG21	1:D:302:LEU:HD13	1.85	0.58
1:B:33:LEU:O	1:B:50:ARG:NH2	2.37	0.57
1:C:102:ARG:N	1:C:220:GLN:NE2	2.52	0.57
1:C:14:ARG:HA	1:C:315:ASP:OD2	2.05	0.57
1:F:30:ILE:HG12	1:F:54:PHE:HD1	1.68	0.57
1:F:6:ASP:O	1:F:8:ASN:N	2.37	0.57
1:C:27:ASN:HB3	1:C:60:THR:HG21	1.84	0.57
1:F:199:ARG:HH22	1:F:217:LYS:HD2	1.69	0.57
1:C:256:GLY:HA3	1:C:332:ASN:O	2.05	0.57
1:E:277:ASN:CB	1:E:334:ASN:HD22	2.16	0.57
1:A:138:PHE:HB3	1:A:149:TYR:CD2	2.39	0.57
1:B:111:LEU:HD21	1:B:122:MET:HE3	1.85	0.57
1:C:207:PHE:CZ	1:C:391:ASP:HB2	2.40	0.57
1:E:385:ARG:HH11	1:E:385:ARG:HB3	1.69	0.57
1:D:59:ASN:HD22	1:D:195:ILE:HD12	1.69	0.57
1:A:79:ARG:HE	1:A:94:ASN:HD21	1.53	0.57
1:E:218:ASN:ND2	1:E:220:ARG:HB2	2.19	0.57
1:F:214:THR:OG1	1:F:216:GLU:HG2	2.03	0.57
1:B:220:ARG:HH22	1:B:255:ASP:CG	2.08	0.57
1:D:13:PHE:HB2	1:D:316:VAL:HB	1.86	0.57
1:A:39:ARG:HG2	1:A:39:ARG:HH11	1.68	0.57
1:C:58:PRO:HD3	1:C:119:ASN:ND2	2.20	0.57
1:B:79:ARG:NH1	1:B:94:ASN:ND2	2.50	0.57
1:A:35:ARG:N	1:A:50:ARG:HH22	2.02	0.57
1:D:384:GLN:NE2	1:D:386:GLU:HB2	2.20	0.57
1:F:362:GLU:O	1:F:366:GLN:HG3	2.05	0.57
1:E:87:ASN:HD22	1:E:88:ASP:H	1.53	0.57
1:B:247:LEU:O	1:B:249:ILE:HG13	2.04	0.57
1:C:319:ILE:N	1:C:319:ILE:HD12	2.19	0.57
1:C:32:LEU:CD1	1:C:50:ARG:HH22	2.18	0.57
1:F:151:GLN:HG2	1:F:174:PHE:CZ	2.40	0.56
1:D:50:ARG:NH2	2:D:446:HOH:O	2.35	0.56
1:F:306:ARG:HD3	1:F:308:ARG:NH1	2.19	0.56
1:E:206:SER:H	1:E:209:THR:HG22	1.70	0.56
1:E:132:PRO:HA	2:E:442:HOH:O	2.06	0.56
1:F:32:LEU:HD22	1:F:50:ARG:NH2	2.20	0.56
1:E:207:ARG:NH2	1:E:222:ARG:HA	2.19	0.56
1:F:254:ASN:HB3	1:F:334:ASN:O	2.06	0.56
1:A:356:ASN:HD22	1:A:359:ARG:CD	2.19	0.56
1:E:375:GLN:O	1:E:379:ARG:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:LEU:HD21	1:F:323:TYR:HB3	1.88	0.56
1:E:219:LEU:H	1:E:219:LEU:HD23	1.69	0.56
1:F:195:ASN:ND2	1:F:198:SER:N	2.54	0.56
1:F:9:ASN:ND2	1:F:11:PHE:H	2.03	0.56
1:F:32:LEU:HD21	1:F:50:ARG:HD2	1.88	0.56
1:D:319:ILE:HD12	1:D:319:ILE:N	2.21	0.56
1:E:222:ARG:HH22	1:E:240:LYS:HG3	1.69	0.56
1:C:61:ILE:HG13	1:C:111:LEU:O	2.05	0.56
1:B:190:LEU:HD23	1:C:368:LEU:HD21	1.88	0.56
1:C:196:LEU:CD2	1:C:230:SER:HB2	2.35	0.56
1:A:313:GLU:O	1:A:314:ASP:HB2	2.06	0.56
1:C:39:ARG:NH1	1:C:39:ARG:HG2	2.21	0.55
1:E:173:LEU:O	1:F:371:PRO:HD2	2.06	0.55
1:B:4:ARG:HB2	1:B:306:ARG:O	2.06	0.55
1:D:9:ASN:ND2	1:D:11:PHE:H	2.04	0.55
1:C:229:SER:OG	1:C:337:ALA:HB3	2.06	0.55
1:F:207:PHE:CZ	1:F:391:ASP:HB2	2.42	0.55
1:C:302:LEU:HD12	1:C:302:LEU:H	1.72	0.55
1:C:50:ARG:NH2	1:C:50:ARG:HB3	2.14	0.55
1:E:26:GLN:H	1:E:26:GLN:HE21	1.53	0.55
1:C:89:ASP:CG	1:C:90:ARG:H	2.09	0.55
1:B:261:LEU:H	1:B:261:LEU:HD23	1.70	0.55
1:C:35:ARG:CZ	1:C:38:LYS:HG3	2.37	0.55
1:B:37:ASN:H	1:B:37:ASN:ND2	1.98	0.55
1:F:73:LEU:HG	1:F:124:TRP:NE1	2.21	0.55
1:B:218:ASN:HD22	1:B:220:ARG:N	2.05	0.55
1:E:9:ASN:C	1:E:9:ASN:HD22	2.09	0.55
1:C:112:VAL:HG12	1:C:113:ASN:N	2.21	0.55
1:B:265:HIS:HB2	1:B:348:ASN:O	2.07	0.55
1:B:382:LYS:HE2	1:B:385:ARG:CZ	2.37	0.55
1:F:235:GLU:CD	1:F:331:SER:HA	2.27	0.55
1:A:285:LEU:HD22	1:A:286:VAL:N	2.22	0.55
1:A:285:LEU:HD21	1:A:323:TYR:HB3	1.87	0.55
1:B:280:ASP:HB2	1:B:330:THR:OG1	2.06	0.55
1:F:227:PHE:CD2	1:F:227:PHE:C	2.81	0.55
1:B:26:GLN:NE2	1:B:26:GLN:N	2.44	0.55
1:C:207:PHE:HB3	1:C:237:ALA:CB	2.37	0.55
1:B:102:ARG:H	1:B:243:GLN:NE2	2.05	0.55
1:A:37:ASN:H	1:A:37:ASN:ND2	1.98	0.54
1:D:38:LYS:HD3	1:D:39:ARG:N	2.22	0.54
1:C:102:ARG:CB	1:C:220:GLN:HE21	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASN:HA	1:A:195:ILE:CD1	2.36	0.54
1:E:32:LEU:HD11	1:E:50:ARG:NH2	2.21	0.54
1:B:218:ASN:HD22	1:B:220:ARG:H	1.53	0.54
1:A:120:LEU:HD21	1:A:122:MET:CE	2.37	0.54
1:D:237:THR:OG1	1:D:240:LYS:HE2	2.07	0.54
1:D:221:SER:O	1:D:222:ARG:HG3	2.07	0.54
1:F:302:LEU:CD2	1:F:302:LEU:H	2.19	0.54
1:A:356:ASN:HD22	1:A:359:ARG:CG	2.20	0.54
1:B:257:ASN:ND2	1:B:257:ASN:N	2.56	0.54
1:C:378:GLU:HG2	1:C:382:LYS:HG3	1.89	0.54
1:D:365:VAL:HG21	1:F:110:TYR:CE2	2.42	0.54
1:E:270:ALA:H	1:E:345:ASN:ND2	2.04	0.54
1:C:56:SER:OG	1:C:120:LEU:HB3	2.07	0.54
1:F:170:ASN:ND2	1:F:175:GLY:H	2.06	0.54
1:A:224:PRO:HG2	1:A:227:SER:HB2	1.90	0.54
1:E:219:LEU:HB2	1:E:236:ILE:HD11	1.89	0.54
1:A:29:ARG:HD3	1:A:31:ARG:CG	2.34	0.54
1:F:382:LYS:NZ	1:F:385:ARG:HH21	2.05	0.54
1:F:102:ARG:H	1:F:220:GLN:NE2	2.06	0.54
1:E:85:VAL:HG23	1:F:360:GLN:HB3	1.88	0.54
1:F:9:ASN:C	1:F:9:ASN:ND2	2.61	0.54
1:E:385:ARG:HB3	1:E:385:ARG:NH1	2.22	0.54
1:C:166:PHE:CD2	1:C:169:ILE:HD11	2.43	0.54
1:E:241:ASN:OD1	1:E:243:GLN:HB2	2.07	0.54
1:E:50:ARG:NH1	2:E:450:HOH:O	2.41	0.54
1:B:31:ARG:HE	1:B:53:GLN:NE2	2.05	0.54
1:B:215:GLU:HB3	1:B:216:PRO:HD2	1.90	0.54
1:F:80:ALA:O	1:F:95:LEU:N	2.40	0.54
1:E:261:LEU:HD22	1:E:392:ALA:HB2	1.89	0.54
1:C:205:ASN:ND2	1:C:389:PHE:HB2	2.23	0.54
1:B:313:GLU:O	1:B:314:ASP:HB2	2.08	0.53
1:B:219:LEU:HD23	1:B:253:SER:HB2	1.91	0.53
1:E:102:ARG:CB	1:E:243:GLN:HE21	2.18	0.53
1:F:260:ILE:CD1	1:F:311:LEU:HD11	2.38	0.53
1:D:55:GLN:HA	1:D:120:LEU:O	2.08	0.53
1:B:110:TYR:CE2	1:C:365:VAL:HG21	2.43	0.53
1:C:246:LYS:H	1:C:345:ASN:HD22	1.57	0.53
1:B:219:LEU:HD21	1:B:253:SER:N	2.23	0.53
1:C:33:LEU:O	1:C:50:ARG:NH2	2.42	0.53
1:E:218:ASN:HD22	1:E:220:ARG:N	2.00	0.53
1:B:159:GLU:OE2	1:B:166:PHE:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:LYS:H	1:F:345:ASN:HD22	1.57	0.53
1:A:224:PRO:HD3	1:A:234:PHE:CE2	2.44	0.53
1:D:73:LEU:HD22	1:D:124:TRP:CG	2.43	0.53
1:B:102:ARG:H	1:B:243:GLN:HE22	1.57	0.53
1:C:202:ILE:HG12	1:C:210:PHE:O	2.09	0.53
1:C:54:PHE:HE2	1:C:120:LEU:HD23	1.74	0.53
1:F:218:ASN:HB3	1:F:221:LEU:HB2	1.91	0.53
1:F:151:GLN:HG2	1:F:174:PHE:CE1	2.43	0.53
1:D:222:ARG:NH2	1:D:222:ARG:HG3	2.23	0.53
1:F:143:THR:HG21	1:F:185:GLY:O	2.09	0.53
1:A:189:GLU:C	1:A:190:LEU:HD12	2.29	0.52
1:D:237:THR:H	1:D:240:LYS:CE	2.21	0.52
1:F:386:GLU:HB3	1:F:390:VAL:HG12	1.91	0.52
1:F:25:ASN:OD1	1:F:27:ASN:N	2.42	0.52
1:C:240:LEU:HD12	1:C:388:TYR:N	2.23	0.52
1:B:274:LEU:HD22	1:B:335:PHE:CD2	2.44	0.52
1:D:274:LEU:C	1:D:274:LEU:HD12	2.30	0.52
1:D:110:TYR:CE2	1:E:365:VAL:HG21	2.43	0.52
1:C:39:ARG:HD2	1:C:40:SER:OG	2.10	0.52
1:B:283:ILE:CD1	1:B:311:LEU:HD11	2.39	0.52
1:E:269:LYS:H	1:E:345:ASN:ND2	2.07	0.52
1:C:258:ALA:HB2	1:C:333:LEU:HD22	1.90	0.52
1:C:15:SER:HB2	1:C:31:ARG:HH12	1.75	0.52
1:E:110:TYR:CE2	1:F:365:VAL:HG21	2.44	0.52
1:F:115:HIS:CE1	1:F:118:GLN:H	2.27	0.52
1:C:62:LEU:HD23	1:C:186:VAL:O	2.09	0.52
1:A:277:ASN:ND2	1:A:277:ASN:O	2.43	0.52
1:D:140:LEU:HD11	1:E:358:VAL:HG22	1.91	0.52
1:A:285:LEU:HD22	1:A:286:VAL:H	1.73	0.52
1:B:208:LYS:HG3	1:B:208:LYS:O	2.10	0.52
1:A:218:ASN:HD22	1:A:220:ARG:N	2.02	0.52
1:B:258:GLU:H	1:B:332:ASN:ND2	2.08	0.52
1:C:247:ALA:H	1:C:345:ASN:ND2	2.08	0.52
1:F:189:GLU:O	1:F:190:LEU:HD23	2.10	0.52
1:B:222:ARG:HH22	1:B:240:LYS:HG3	1.74	0.52
1:F:251:LEU:HD12	1:F:251:LEU:C	2.30	0.52
1:E:6:ASP:O	1:E:7:GLU:HB2	2.09	0.52
1:C:146:GLN:NE2	1:C:146:GLN:C	2.63	0.52
1:C:147:GLN:HB3	1:C:151:GLN:OE1	2.10	0.52
1:D:261:LEU:HD22	1:D:392:ALA:HB2	1.92	0.52
1:D:10:PRO:HB2	1:D:40:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASN:N	1:D:223:ASN:HD22	2.08	0.52
1:D:34:GLN:HE22	1:D:38:LYS:HE2	1.75	0.51
1:B:6:ASP:O	1:B:7:GLU:CB	2.58	0.51
1:A:58:PRO:HD3	1:A:119:ASN:ND2	2.24	0.51
1:D:207:ARG:HG3	1:D:207:ARG:NH1	2.25	0.51
1:A:69:ALA:CB	1:A:128:PRO:HA	2.40	0.51
1:A:373:SER:H	1:A:376:ASP:HB2	1.75	0.51
1:B:68:ASP:OD2	1:B:135:TYR:HB2	2.09	0.51
1:F:240:LEU:HD13	1:F:351:ALA:O	2.10	0.51
1:B:170:ASN:O	1:B:175:GLY:N	2.42	0.51
1:F:380:LEU:C	1:F:382:LYS:H	2.14	0.51
1:A:67:ALA:C	1:A:69:ALA:H	2.14	0.51
1:A:170:ASN:ND2	1:A:174:PHE:HB2	2.26	0.51
1:C:385:ARG:HH11	1:C:385:ARG:HG2	1.75	0.51
1:C:320:PRO:HB2	1:C:323:TYR:CD1	2.45	0.51
1:E:377:VAL:O	1:E:381:LEU:HG	2.10	0.51
1:B:331:SER:O	1:B:332:ASN:C	2.49	0.51
1:F:30:ILE:HG12	1:F:54:PHE:CD1	2.45	0.51
1:E:193:GLU:OE2	1:E:196:ARG:NH1	2.43	0.51
1:D:38:LYS:HD3	1:D:38:LYS:C	2.30	0.51
1:E:277:ASN:HB3	1:E:334:ASN:ND2	2.22	0.51
1:E:387:SER:O	1:E:389:PHE:N	2.40	0.51
1:C:189:GLU:H	1:C:189:GLU:CD	2.13	0.51
1:B:59:ASN:HA	1:B:195:ILE:HD11	1.92	0.51
1:E:259:GLY:O	1:E:392:ALA:HB3	2.10	0.51
1:E:250:PHE:C	1:E:250:PHE:CD2	2.84	0.51
1:D:17:ASN:HD22	1:D:18:SER:N	2.08	0.51
1:B:382:LYS:NZ	1:B:385:ARG:HH12	2.06	0.51
1:F:48:ASP:OD1	1:F:132:PRO:HB3	2.11	0.51
1:B:30:ILE:HG12	1:B:54:PHE:HD1	1.77	0.51
1:B:364:GLN:CD	1:B:364:GLN:H	2.14	0.51
1:E:219:LEU:HB3	1:E:236:ILE:HG12	1.93	0.50
1:A:35:ARG:HG3	1:A:50:ARG:HH22	1.74	0.50
1:F:49:TYR:O	1:F:50:ARG:HG2	2.11	0.50
1:D:130:ASN:C	1:E:45:ASN:HD22	2.15	0.50
1:F:169:ILE:HG13	1:F:170:ASN:N	2.26	0.50
1:F:119:ASN:HD22	1:F:119:ASN:N	2.09	0.50
1:E:122:MET:HE1	1:E:124:TRP:HE1	1.75	0.50
1:C:102:ARG:H	1:C:220:GLN:HE22	1.59	0.50
1:F:189:GLU:O	1:F:190:LEU:O	2.30	0.50
1:F:242:HIS:HB3	1:F:349:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:ARG:CG	1:F:16:SER:HB3	2.38	0.50
1:C:99:ASP:HA	1:C:195:ASN:HA	1.94	0.50
1:D:274:LEU:C	1:D:274:LEU:CD1	2.80	0.50
1:E:258:GLU:H	1:E:332:ASN:ND2	2.10	0.50
1:E:331:SER:O	1:E:332:ASN:C	2.50	0.50
1:C:80:ALA:HB2	1:C:120:LEU:CD1	2.41	0.50
1:C:266:LYS:HB3	1:C:303:GLU:HB2	1.93	0.50
1:C:215:PRO:HD2	1:C:216:GLU:OE1	2.12	0.50
1:E:57:LYS:HB3	1:E:58:PRO:HD2	1.93	0.50
1:A:363:ARG:HG2	1:A:378:GLU:OE1	2.11	0.50
1:B:9:ASN:C	1:B:9:ASN:HD22	2.12	0.50
1:B:168:GLU:O	1:B:172:VAL:HG23	2.12	0.50
1:F:89:ASP:CG	1:F:90:ARG:N	2.65	0.50
1:C:61:ILE:HG13	1:C:112:VAL:HG22	1.93	0.49
1:F:261:GLU:HB2	1:F:326:VAL:HG12	1.94	0.49
1:D:9:ASN:HD22	1:D:11:PHE:H	1.60	0.49
1:A:176:GLU:HB2	2:A:444:HOH:O	2.12	0.49
1:C:34:GLN:OE1	1:C:39:ARG:HG2	2.12	0.49
1:D:34:GLN:NE2	1:D:38:LYS:HE2	2.27	0.49
1:B:312:SER:O	1:B:315:ASP:HB2	2.12	0.49
1:A:267:ASN:HB3	1:A:345:ASN:HD21	1.77	0.49
1:A:222:ARG:NH2	1:A:222:ARG:HG3	2.27	0.49
1:B:379:ARG:HH11	1:B:379:ARG:HG3	1.77	0.49
1:F:196:LEU:HD21	1:F:230:SER:N	2.27	0.49
1:D:67:ALA:C	1:D:69:ALA:H	2.16	0.49
1:E:230:PHE:CZ	1:E:391:ASP:HB2	2.47	0.49
1:B:363:ARG:HH11	1:B:363:ARG:HG2	1.76	0.49
1:D:244:LEU:HG	1:D:249:ILE:O	2.12	0.49
1:C:79:ARG:HD2	1:C:94:ASN:ND2	2.24	0.49
1:E:102:ARG:H	1:E:243:GLN:HE22	1.61	0.49
1:F:205:ASN:ND2	1:F:389:PHE:HB2	2.27	0.49
1:F:101:GLN:HG2	1:F:102:ARG:N	2.27	0.49
1:F:32:LEU:HD22	1:F:50:ARG:HH21	1.78	0.49
1:E:222:ARG:NH1	1:E:236:ILE:HD12	2.27	0.49
1:A:380:LEU:HD12	1:C:172:VAL:HB	1.94	0.49
1:E:269:LYS:H	1:E:345:ASN:HD22	1.60	0.49
1:D:224:PRO:HG2	1:D:227:SER:HB2	1.93	0.49
1:F:347:ARG:NH1	2:F:417:HOH:O	2.41	0.49
1:F:331:SER:O	1:F:332:ASN:C	2.50	0.49
1:A:53:GLN:HE22	1:A:314:ASP:HB3	1.77	0.49
1:C:216:GLU:H	1:C:216:GLU:CD	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:PRO:HB3	1:B:245:ARG:HA	1.93	0.49
1:F:234:ASN:N	1:F:234:ASN:ND2	2.59	0.49
1:B:87:ASN:HD22	1:B:88:ASP:H	1.59	0.49
1:F:89:ASP:OD1	1:F:90:ARG:N	2.45	0.49
1:A:9:ASN:HD22	1:A:9:ASN:C	2.15	0.49
1:E:247:LEU:O	1:E:249:ILE:HG13	2.13	0.49
1:E:219:LEU:HA	1:E:236:ILE:HD11	1.94	0.49
1:F:14:ARG:C	1:F:16:SER:H	2.16	0.49
1:B:250:PHE:CD2	1:B:250:PHE:C	2.86	0.49
1:E:284:GLU:HB2	1:E:326:VAL:CG1	2.43	0.49
1:E:321:ALA:O	1:E:322:ALA:HB3	2.13	0.49
1:D:184:GLU:HG3	2:D:450:HOH:O	2.11	0.49
1:C:364:GLN:CD	1:C:364:GLN:H	2.17	0.49
1:A:147:GLN:OE1	1:B:304:VAL:HG22	2.13	0.49
1:C:386:GLU:CB	1:C:390:VAL:HG12	2.38	0.48
1:A:59:ASN:ND2	1:A:195:ILE:HD12	2.27	0.48
1:B:277:ASN:CB	1:B:334:ASN:HD22	2.26	0.48
1:A:131:LYS:HG3	1:A:134:ARG:HB2	1.94	0.48
1:D:17:ASN:C	1:D:17:ASN:ND2	2.64	0.48
1:E:9:ASN:ND2	1:E:11:PHE:H	2.12	0.48
1:C:205:ASN:HD21	1:C:389:PHE:HB2	1.78	0.48
1:C:238:LEU:HD21	1:C:390:VAL:HG22	1.96	0.48
1:A:55:GLN:HA	1:A:120:LEU:O	2.13	0.48
1:C:61:ILE:CG1	1:C:112:VAL:HG22	2.43	0.48
1:F:189:GLU:O	1:F:190:LEU:C	2.52	0.48
1:F:60:THR:O	1:F:112:VAL:HG13	2.13	0.48
1:F:261:GLU:HB2	1:F:326:VAL:CG1	2.43	0.48
1:A:270:ALA:H	1:A:345:ASN:ND2	2.09	0.48
1:F:125:LEU:HD22	1:F:338:PHE:CD2	2.49	0.48
1:D:192:LYS:O	1:D:196:ARG:HB2	2.13	0.48
1:D:322:ALA:HB3	1:F:68:ASP:HB3	1.94	0.48
1:F:215:PRO:O	1:F:222:ARG:HB2	2.13	0.48
1:D:40:SER:C	1:D:42:GLN:H	2.15	0.48
1:C:190:LEU:HD23	1:C:190:LEU:O	2.14	0.48
1:B:363:ARG:NH1	1:B:378:GLU:OE2	2.47	0.48
1:E:101:GLN:NE2	1:E:216:PRO:HD3	2.29	0.48
1:F:225:ASP:OD2	1:F:343:GLU:HB2	2.13	0.48
1:F:80:ALA:HB2	1:F:120:LEU:CD1	2.44	0.48
1:F:254:ASN:O	1:F:313:GLU:HG3	2.14	0.48
1:E:160:THR:HG21	1:F:392:ALA:HA	1.96	0.48
1:C:59:ASN:HD21	1:C:116:ASP:CG	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LEU:HB3	1:C:125:LEU:HB3	1.95	0.48
1:D:10:PRO:HB2	1:D:40:SER:CB	2.44	0.47
1:A:223:ASN:N	1:A:223:ASN:HD22	2.11	0.47
1:F:13:PHE:CZ	1:F:39:ARG:HG3	2.49	0.47
1:B:81:ILE:HD11	1:B:199:SER:HB3	1.94	0.47
1:F:15:SER:CB	1:F:314:ASP:HB3	2.44	0.47
1:B:49:TYR:O	1:B:50:ARG:HG2	2.14	0.47
1:A:359:ARG:HH11	1:A:359:ARG:HB2	1.79	0.47
1:F:253:ILE:HD11	1:F:311:LEU:CD1	2.44	0.47
1:A:288:ILE:HG21	1:A:302:LEU:HD13	1.95	0.47
1:F:191:ASP:OD2	1:F:192:GLU:N	2.46	0.47
1:C:100:ALA:HB3	1:C:194:PHE:CE2	2.49	0.47
1:E:261:LEU:N	1:E:261:LEU:HD23	2.29	0.47
1:A:139:PHE:CE2	1:A:186:VAL:HB	2.49	0.47
1:D:131:LYS:HG3	1:D:134:ARG:HB2	1.96	0.47
1:C:306:ARG:HB3	1:C:308:ARG:HH11	1.79	0.47
1:D:378:GLU:O	1:D:382:LYS:HB2	2.14	0.47
1:B:319:ILE:HD12	1:B:319:ILE:N	2.29	0.47
1:D:57:LYS:HB3	1:D:58:PRO:HD2	1.97	0.47
1:C:76:LEU:HD11	1:C:123:ILE:HG12	1.95	0.47
1:C:85:VAL:HG13	1:C:108:THR:HB	1.96	0.47
1:B:37:ASN:N	1:B:37:ASN:ND2	2.61	0.47
1:B:214:ASP:OD1	1:B:215:GLU:HG3	2.14	0.47
1:F:73:LEU:HG	1:F:124:TRP:CD1	2.50	0.47
1:E:32:LEU:HD23	1:E:52:VAL:HG22	1.96	0.47
1:D:359:ARG:HH11	1:D:382:LYS:HD2	1.80	0.47
1:C:259:ASN:ND2	1:C:330:THR:CG2	2.78	0.47
1:E:80:ALA:HB2	1:E:120:LEU:HD22	1.97	0.47
1:F:71:PHE:HE2	1:F:126:ALA:HB2	1.80	0.47
1:F:85:VAL:CG1	1:F:108:THR:HG22	2.44	0.47
1:F:384:GLN:NE2	1:F:386:GLU:HB2	2.29	0.47
1:B:382:LYS:HG3	1:B:385:ARG:NH1	2.29	0.47
1:D:306:ARG:NH2	2:D:480:HOH:O	2.48	0.47
1:A:59:ASN:CA	1:A:195:ILE:HD11	2.42	0.47
1:F:257:ASP:O	1:F:258:ALA:HB2	2.14	0.47
1:E:306:ARG:HD3	2:E:451:HOH:O	2.14	0.47
1:A:210:ILE:HD11	1:A:236:ILE:CG2	2.45	0.47
1:F:357:VAL:O	1:F:360:GLN:HB2	2.15	0.47
1:E:189:GLU:C	1:E:190:LEU:HG	2.35	0.47
1:A:249:ILE:HA	1:A:339:GLY:O	2.14	0.47
1:A:73:LEU:HD22	1:A:124:TRP:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:GLU:HG2	1:F:188:VAL:HG12	1.96	0.47
1:A:217:PHE:CD1	1:A:217:PHE:N	2.82	0.47
1:B:23:PHE:CD2	1:B:186:VAL:HG22	2.50	0.47
1:A:356:ASN:HD22	1:A:359:ARG:HD3	1.78	0.47
1:F:256:GLY:HA3	1:F:332:ASN:O	2.15	0.47
1:B:267:ASN:HB3	1:B:345:ASN:HD21	1.79	0.47
1:F:247:ALA:H	1:F:345:ASN:ND2	2.12	0.47
1:A:250:PHE:CD2	1:A:250:PHE:C	2.87	0.47
1:E:219:LEU:CB	1:E:236:ILE:HD11	2.45	0.47
1:D:356:ASN:HD22	1:D:356:ASN:C	2.18	0.47
1:C:320:PRO:HB2	1:C:323:TYR:CG	2.50	0.47
1:B:83:THR:HG21	1:B:110:TYR:CE2	2.50	0.47
1:C:258:ALA:CB	1:C:333:LEU:HD22	2.45	0.47
1:D:69:ALA:O	1:D:105:ALA:HA	2.15	0.47
1:B:154:SER:OG	1:B:157:ILE:HD13	2.14	0.47
1:E:319:ILE:HG21	1:E:325:PHE:CD1	2.50	0.47
1:F:266:LYS:HB3	1:F:303:GLU:HB2	1.97	0.47
1:C:54:PHE:CD2	1:C:122:MET:HE2	2.49	0.47
1:D:9:ASN:ND2	1:D:9:ASN:C	2.68	0.47
1:D:285:LEU:HD22	1:D:286:VAL:N	2.30	0.47
1:B:281:ALA:HB2	1:B:333:LEU:HD22	1.97	0.47
1:C:266:LYS:HE3	1:C:305:GLN:OE1	2.14	0.47
1:F:61:ILE:HB	1:F:112:VAL:HG22	1.97	0.47
1:B:165:GLU:HG3	1:B:167:GLU:HG3	1.96	0.47
1:F:55:GLN:HA	1:F:120:LEU:O	2.14	0.46
1:C:73:LEU:HG	1:C:124:TRP:NE1	2.29	0.46
1:F:321:ALA:O	1:F:322:ALA:HB3	2.14	0.46
1:C:64:PRO:HG3	1:C:110:TYR:CD1	2.50	0.46
1:A:371:PRO:O	1:A:372:GLY:O	2.33	0.46
1:A:356:ASN:HD22	1:A:359:ARG:HG2	1.79	0.46
1:F:353:GLU:OE2	1:F:385:ARG:HA	2.15	0.46
1:B:34:GLN:HE21	1:B:39:ARG:HB2	1.80	0.46
1:D:59:ASN:HA	1:D:195:ILE:CD1	2.45	0.46
1:D:380:LEU:HD11	1:F:169:ILE:HA	1.96	0.46
1:F:32:LEU:CD2	1:F:50:ARG:HD2	2.45	0.46
1:E:260:ALA:HA	1:E:392:ALA:H	1.80	0.46
1:C:385:ARG:HG2	1:C:385:ARG:NH1	2.28	0.46
1:C:111:LEU:HD21	1:C:120:LEU:HD21	1.97	0.46
1:E:154:SER:HB3	1:F:308:ARG:NH2	2.31	0.46
1:A:79:ARG:HB2	1:A:115:HIS:CE1	2.51	0.46
1:A:110:TYR:CE2	1:B:365:VAL:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LEU:HD12	1:C:34:GLN:H	1.81	0.46
1:C:260:ILE:O	1:C:308:ARG:HA	2.15	0.46
1:D:356:ASN:HB3	1:D:359:ARG:HG2	1.96	0.46
1:D:13:PHE:HB2	1:D:316:VAL:O	2.15	0.46
1:F:33:LEU:O	1:F:50:ARG:NH2	2.39	0.46
1:C:15:SER:HB3	1:C:314:ASP:O	2.15	0.46
2:A:430:HOH:O	1:B:45:ASN:HB2	2.14	0.46
1:C:58:PRO:HB3	1:C:116:ASP:HA	1.97	0.46
1:A:47:ARG:HH12	1:A:132:PRO:CB	2.28	0.46
1:B:79:ARG:HB2	1:B:115:HIS:NE2	2.31	0.46
1:C:362:GLU:O	1:C:366:GLN:HG3	2.16	0.46
1:F:170:ASN:HD22	1:F:175:GLY:H	1.62	0.46
1:C:215:PRO:HB3	1:C:222:ARG:HA	1.97	0.46
1:A:222:ARG:HG3	1:A:222:ARG:HH21	1.80	0.46
1:F:82:LEU:HD13	1:F:111:LEU:HD13	1.97	0.46
1:E:19:PHE:CZ	1:E:33:LEU:HD13	2.51	0.46
1:E:33:LEU:O	1:E:50:ARG:NH2	2.48	0.46
1:F:147:GLN:HG2	1:F:151:GLN:OE1	2.16	0.46
1:C:257:ASP:O	1:C:333:LEU:HD13	2.16	0.46
1:D:392:ALA:HA	1:F:160:THR:HG21	1.98	0.46
1:D:80:ALA:HB2	1:D:120:LEU:CD1	2.46	0.46
1:E:129:VAL:O	1:F:45:ASN:ND2	2.48	0.46
1:C:235:GLU:HG2	1:C:236:GLY:N	2.31	0.46
1:F:226:ILE:HA	1:F:339:GLY:O	2.16	0.46
1:B:304:VAL:O	1:B:304:VAL:HG23	2.16	0.46
1:A:7:GLU:OE2	1:A:14:ARG:NH1	2.49	0.46
1:A:200:ARG:O	1:A:201:ARG:HB3	2.14	0.46
1:F:14:ARG:HA	1:F:315:ASP:OD2	2.15	0.46
1:C:82:LEU:HD13	1:C:111:LEU:HD13	1.98	0.46
1:D:206:SER:O	1:D:207:ARG:C	2.54	0.46
1:D:274:LEU:HD22	1:D:335:PHE:CE2	2.51	0.46
1:B:206:SER:O	1:B:209:THR:HG22	2.16	0.46
1:E:166:PHE:HZ	1:E:170:ASN:HD22	1.61	0.46
1:A:319:ILE:HD13	1:A:325:PHE:CZ	2.52	0.46
1:C:377:VAL:O	1:C:381:LEU:HG	2.17	0.45
1:E:196:ARG:C	1:E:198:LEU:H	2.19	0.45
1:D:267:ASN:HB3	1:D:345:ASN:HD21	1.81	0.45
1:F:31:ARG:HH21	1:F:53:GLN:CD	2.20	0.45
1:F:87:ASN:HD22	1:F:87:ASN:C	2.20	0.45
1:D:23:PHE:HZ	1:D:185:GLY:HA3	1.81	0.45
1:C:111:LEU:HD21	1:C:122:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:PHE:CD2	1:F:169:ILE:HD11	2.51	0.45
1:D:320:PRO:HB2	1:D:323:TYR:CD1	2.51	0.45
1:A:210:ILE:HD11	1:A:236:ILE:HG23	1.99	0.45
1:B:30:ILE:HG12	1:B:54:PHE:CD1	2.52	0.45
1:E:68:ASP:OD2	1:E:135:TYR:HB2	2.16	0.45
1:D:226:TYR:HB3	1:D:388:TYR:CD1	2.51	0.45
1:D:122:MET:HE3	1:D:124:TRP:HE1	1.82	0.45
1:E:277:ASN:ND2	2:E:460:HOH:O	2.50	0.45
1:F:170:ASN:C	1:F:170:ASN:HD22	2.19	0.45
1:A:384:GLN:NE2	1:A:386:GLU:HB2	2.32	0.45
1:C:261:GLU:CD	1:C:308:ARG:HH21	2.20	0.45
1:E:167:GLU:HG3	1:E:168:GLU:N	2.31	0.45
1:D:274:LEU:HD22	1:D:335:PHE:CD2	2.52	0.45
1:B:168:GLU:CD	1:C:383:LYS:HZ2	2.20	0.45
1:A:183:GLN:CG	1:A:188:VAL:CG1	2.91	0.45
1:E:222:ARG:CZ	1:E:236:ILE:HD12	2.47	0.45
1:E:235:GLU:C	1:E:236:ILE:HD13	2.37	0.45
1:F:215:PRO:HB3	1:F:222:ARG:HA	1.99	0.45
1:E:319:ILE:N	1:E:319:ILE:HD12	2.30	0.45
1:E:6:ASP:HB2	1:E:7:GLU:OE1	2.17	0.45
1:A:150:LEU:HD21	1:B:350:LEU:HD13	1.99	0.45
1:E:49:TYR:CZ	1:E:340:ILE:HD12	2.52	0.45
1:A:120:LEU:HD21	1:A:122:MET:HE2	1.98	0.45
1:B:6:ASP:OD1	1:B:6:ASP:O	2.35	0.45
1:E:6:ASP:C	1:E:8:ASN:H	2.19	0.45
1:B:23:PHE:CD1	1:B:24:GLU:N	2.85	0.45
1:C:81:ILE:HG13	1:C:114:PRO:HG3	1.98	0.45
1:E:30:ILE:HG12	1:E:54:PHE:HD1	1.81	0.45
1:C:65:HIS:HB2	1:C:138:PHE:O	2.17	0.45
1:E:226:TYR:HB2	1:E:233:PHE:HB3	1.99	0.45
1:F:229:SER:OG	1:F:337:ALA:HB3	2.17	0.45
1:D:304:VAL:O	1:D:304:VAL:HG23	2.17	0.45
1:A:74:PHE:HE2	1:A:219:LEU:HD13	1.81	0.45
1:C:119:ASN:N	1:C:119:ASN:ND2	2.65	0.45
1:B:85:VAL:HG13	1:B:108:THR:HB	1.98	0.45
1:E:73:LEU:HG	1:E:124:TRP:CD1	2.52	0.45
1:A:120:LEU:HD21	1:A:122:MET:HE1	1.98	0.45
1:F:214:THR:H	1:F:217:LYS:HE3	1.81	0.45
1:B:32:LEU:CD1	1:B:50:ARG:CZ	2.92	0.45
1:D:40:SER:C	1:D:42:GLN:N	2.70	0.45
1:C:76:LEU:HB2	1:C:121:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:HIS:HB2	1:E:348:ASN:O	2.16	0.45
1:D:217:PHE:N	1:D:217:PHE:CD1	2.85	0.45
1:D:37:ASN:HD22	1:D:37:ASN:N	2.12	0.44
1:D:114:PRO:HA	1:D:195:ILE:HD13	1.98	0.44
1:F:37:ASN:H	1:F:37:ASN:ND2	2.12	0.44
1:C:387:SER:O	1:C:389:PHE:N	2.44	0.44
1:A:217:PHE:CZ	1:A:244:LEU:HD13	2.52	0.44
1:C:238:LEU:HD21	1:C:390:VAL:CG2	2.48	0.44
1:D:261:LEU:N	1:D:261:LEU:HD23	2.31	0.44
1:E:162:PHE:HB2	1:E:169:ILE:CD1	2.47	0.44
1:E:258:GLU:H	1:E:332:ASN:HD22	1.63	0.44
1:B:148:SER:OG	1:B:150:LEU:HB2	2.18	0.44
1:F:141:SER:O	1:F:148:SER:HB2	2.18	0.44
1:B:169:ILE:HA	1:C:380:LEU:HD11	2.00	0.44
1:B:184:GLU:O	1:B:185:GLY:O	2.36	0.44
1:B:387:SER:O	1:B:389:PHE:N	2.48	0.44
1:A:22:LEU:HD21	1:A:32:LEU:HD12	1.99	0.44
1:B:32:LEU:HD23	1:B:52:VAL:HG22	1.99	0.44
1:F:58:PRO:HD3	1:F:119:ASN:ND2	2.31	0.44
1:A:224:PRO:CG	1:A:227:SER:HB2	2.46	0.44
1:D:79:ARG:HB2	1:D:115:HIS:CE1	2.53	0.44
1:D:8:ASN:ND2	1:D:8:ASN:O	2.50	0.44
1:F:96:HIS:O	1:F:99:ASP:HB2	2.17	0.44
1:A:357:VAL:O	1:A:360:GLN:HB2	2.17	0.44
1:E:364:GLN:O	1:E:367:GLU:HB3	2.18	0.44
1:A:87:ASN:HD22	1:A:87:ASN:C	2.18	0.44
1:D:306:ARG:HH21	1:D:306:ARG:HG3	1.82	0.44
1:F:37:ASN:ND2	1:F:37:ASN:N	2.65	0.44
1:D:87:ASN:HD22	1:D:87:ASN:C	2.20	0.44
1:B:206:SER:O	1:B:208:LYS:N	2.51	0.44
1:D:263:LEU:HD13	1:D:351:ALA:O	2.17	0.44
1:B:59:ASN:HA	1:B:195:ILE:CD1	2.47	0.44
1:E:219:LEU:HB3	1:E:236:ILE:CG1	2.47	0.44
1:D:261:LEU:HD21	1:D:390:VAL:HG23	1.95	0.44
1:D:85:VAL:CG2	1:E:360:GLN:HB2	2.45	0.44
1:F:87:ASN:HD22	1:F:88:ASP:N	2.16	0.44
1:A:281:ALA:HB2	1:A:333:LEU:HD22	2.00	0.44
1:E:88:ASP:O	1:E:89:ASP:HB3	2.17	0.44
1:B:274:LEU:HD22	1:B:335:PHE:CE2	2.53	0.44
1:D:69:ALA:HB2	1:D:128:PRO:HA	2.00	0.44
1:E:80:ALA:HB2	1:E:120:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:PHE:CZ	1:E:170:ASN:ND2	2.85	0.44
1:E:13:PHE:HB2	1:E:316:VAL:HB	2.00	0.44
1:E:111:LEU:CD2	1:E:122:MET:HE2	2.34	0.44
1:C:58:PRO:HB3	1:C:115:HIS:O	2.18	0.44
1:B:220:ARG:NH2	1:B:255:ASP:OD2	2.51	0.44
1:D:172:VAL:HG22	1:E:376:ASP:HB3	2.00	0.44
1:C:22:LEU:HB2	1:C:30:ILE:O	2.18	0.44
1:E:47:ARG:HH22	1:E:132:PRO:CB	2.31	0.44
1:F:360:GLN:HA	1:F:360:GLN:NE2	2.32	0.44
1:F:12:TYR:O	1:F:39:ARG:NH2	2.50	0.43
1:C:79:ARG:HG2	1:C:80:ALA:N	2.33	0.43
1:B:25:ASN:OD1	1:B:27:ASN:N	2.46	0.43
1:E:254:VAL:HG13	1:E:335:PHE:CE2	2.53	0.43
1:F:79:ARG:HG2	1:F:80:ALA:N	2.33	0.43
1:E:116:ASP:OD2	1:E:192:LYS:HE3	2.19	0.43
1:C:259:ASN:ND2	1:C:330:THR:HG21	2.33	0.43
1:A:171:ARG:HD2	1:A:181:ARG:NH2	2.33	0.43
1:A:361:ILE:CG2	1:A:365:VAL:HB	2.49	0.43
1:E:219:LEU:CA	1:E:236:ILE:HD11	2.48	0.43
1:C:102:ARG:HB3	1:C:220:GLN:NE2	2.33	0.43
1:D:285:LEU:CD2	1:D:323:TYR:HB3	2.45	0.43
1:E:206:SER:O	1:E:209:THR:HG22	2.17	0.43
1:B:206:SER:H	1:B:209:THR:CG2	2.31	0.43
1:C:146:GLN:HE21	1:C:146:GLN:C	2.21	0.43
1:A:387:SER:O	1:A:389:PHE:N	2.43	0.43
1:F:202:ILE:HG12	1:F:210:PHE:O	2.17	0.43
1:C:8:ASN:HD22	1:C:8:ASN:HA	1.52	0.43
1:D:75:VAL:HG21	1:D:95:LEU:HB3	2.00	0.43
1:A:206:SER:O	1:A:207:ARG:C	2.57	0.43
1:D:363:ARG:HG2	1:D:374:ALA:CB	2.46	0.43
1:D:210:ILE:HG23	1:D:211:SER:N	2.32	0.43
1:C:379:ARG:HG3	1:C:379:ARG:NH1	2.31	0.43
1:B:274:LEU:HB3	1:B:317:PHE:O	2.19	0.43
1:E:159:GLU:OE2	1:E:166:PHE:HB2	2.18	0.43
1:D:250:PHE:CD2	1:D:250:PHE:C	2.92	0.43
1:E:122:MET:HE3	1:E:122:MET:HB2	1.76	0.43
1:C:170:ASN:O	1:C:170:ASN:ND2	2.51	0.43
1:B:219:LEU:HD11	1:B:235:GLU:HA	2.00	0.43
1:C:196:LEU:HD13	1:C:213:ILE:HG12	2.00	0.43
1:B:333:LEU:HG	1:B:334:ASN:N	2.33	0.43
1:F:9:ASN:HD21	1:F:11:PHE:HD2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:CE	1:D:124:TRP:HE1	2.32	0.43
1:B:203:LYS:HD3	1:B:215:GLU:OE2	2.18	0.43
1:D:170:ASN:HD22	1:D:174:PHE:HB2	1.84	0.43
1:E:222:ARG:NH1	1:E:236:ILE:CD1	2.82	0.43
1:B:353:GLU:HG3	1:B:385:ARG:O	2.19	0.43
1:F:8:ASN:HA	1:F:8:ASN:HD22	1.59	0.43
1:F:189:GLU:C	1:F:190:LEU:HD23	2.39	0.43
1:F:310:GLU:OE2	1:F:310:GLU:N	2.51	0.43
1:E:59:ASN:CA	1:E:195:ILE:HD11	2.43	0.43
1:A:32:LEU:HD13	1:A:50:ARG:HH11	1.84	0.43
1:E:277:ASN:CB	1:E:334:ASN:ND2	2.81	0.43
1:F:353:GLU:OE1	1:F:382:LYS:HE3	2.18	0.43
1:D:89:ASP:HA	1:E:360:GLN:NE2	2.34	0.43
1:F:25:ASN:OD1	1:F:25:ASN:C	2.58	0.43
1:C:189:GLU:O	1:C:190:LEU:C	2.57	0.43
1:D:321:ALA:O	1:D:322:ALA:HB3	2.18	0.43
1:A:35:ARG:HG2	1:A:50:ARG:NH2	2.32	0.43
1:B:32:LEU:CD2	1:B:52:VAL:HG22	2.48	0.43
1:F:31:ARG:NE	1:F:53:GLN:NE2	2.66	0.43
1:E:364:GLN:O	1:E:368:LEU:HD22	2.19	0.43
1:B:249:ILE:CG2	1:B:250:PHE:N	2.82	0.43
1:C:89:ASP:O	1:C:90:ARG:HB2	2.18	0.43
1:E:85:VAL:HG13	1:E:108:THR:HB	2.01	0.43
1:A:9:ASN:ND2	1:A:11:PHE:H	2.17	0.43
1:F:112:VAL:HG12	1:F:113:ASN:N	2.33	0.43
1:A:284:GLU:HG2	1:A:308:ARG:HG2	2.01	0.43
1:C:242:HIS:HB3	1:C:349:PHE:CD1	2.54	0.43
1:F:380:LEU:C	1:F:380:LEU:HD23	2.39	0.42
1:C:252:VAL:HG21	1:C:336:LEU:HD23	2.01	0.42
1:B:23:PHE:C	1:B:23:PHE:CD1	2.92	0.42
1:B:11:PHE:CE1	1:B:43:LEU:HD21	2.52	0.42
1:B:11:PHE:CD1	1:B:43:LEU:HD21	2.54	0.42
1:A:368:LEU:HD23	1:C:188:VAL:CG2	2.44	0.42
1:F:238:LEU:HD23	1:F:238:LEU:N	2.34	0.42
1:F:261:GLU:HG2	1:F:308:ARG:HE	1.84	0.42
1:F:227:PHE:HD2	1:F:227:PHE:C	2.23	0.42
1:F:61:ILE:CG1	1:F:112:VAL:HG22	2.49	0.42
1:B:282:ASN:OD1	1:B:310:GLU:HG2	2.19	0.42
1:F:6:ASP:C	1:F:8:ASN:N	2.73	0.42
1:B:249:ILE:HG22	1:B:250:PHE:N	2.34	0.42
1:E:5:GLU:O	1:E:6:ASP:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:ILE:N	1:F:319:ILE:HD12	2.34	0.42
1:F:199:ARG:HD3	1:F:213:ILE:CD1	2.49	0.42
1:F:235:GLU:HB2	1:F:332:ASN:N	2.34	0.42
1:C:227:PHE:C	1:C:227:PHE:HD2	2.21	0.42
1:A:362:GLU:HG2	1:C:90:ARG:CZ	2.49	0.42
1:C:330:THR:O	1:C:331:SER:HB3	2.19	0.42
1:A:217:PHE:HZ	1:A:244:LEU:HD13	1.84	0.42
1:D:270:ALA:H	1:D:345:ASN:ND2	2.18	0.42
1:F:65:HIS:HA	1:F:138:PHE:O	2.19	0.42
1:E:146:GLN:NE2	1:E:146:GLN:C	2.73	0.42
1:E:37:ASN:N	1:E:37:ASN:ND2	2.56	0.42
1:F:80:ALA:HB2	1:F:120:LEU:CD2	2.49	0.42
1:B:382:LYS:HG3	1:B:382:LYS:O	2.18	0.42
1:A:23:PHE:CE2	1:A:186:VAL:HG22	2.55	0.42
1:F:71:PHE:CE2	1:F:126:ALA:HB2	2.55	0.42
1:C:384:GLN:HE22	1:C:386:GLU:HB2	1.75	0.42
1:A:351:ALA:N	1:A:356:ASN:OD1	2.52	0.42
1:C:71:PHE:HB2	1:C:103:ILE:HB	2.02	0.42
1:B:269:LYS:H	1:B:345:ASN:ND2	2.16	0.42
1:E:173:LEU:HA	1:F:370:PHE:HB3	2.02	0.42
1:E:305:GLN:NE2	2:E:432:HOH:O	2.52	0.42
1:C:102:ARG:N	1:C:220:GLN:HE21	2.16	0.42
1:A:302:LEU:HG	1:C:23:PHE:CZ	2.54	0.42
1:D:25:ASN:HB3	1:D:27:ASN:H	1.84	0.42
1:D:228:ASN:C	1:D:228:ASN:OD1	2.57	0.42
1:C:32:LEU:CD1	1:C:50:ARG:NH2	2.82	0.42
1:C:13:PHE:CZ	1:C:39:ARG:HG3	2.53	0.42
1:C:35:ARG:HG3	1:C:50:ARG:HE	1.84	0.42
1:F:31:ARG:HH21	1:F:53:GLN:NE2	2.18	0.42
1:F:38:LYS:HA	1:F:38:LYS:HD3	1.92	0.42
1:F:37:ASN:ND2	1:F:38:LYS:H	2.17	0.42
1:D:71:PHE:HA	1:D:125:LEU:O	2.20	0.42
1:D:138:PHE:HB3	1:D:149:TYR:CD2	2.55	0.42
1:A:364:GLN:O	1:A:368:LEU:CD1	2.68	0.42
1:F:254:ASN:C	1:F:254:ASN:HD22	2.23	0.42
1:C:254:ASN:HB3	1:C:334:ASN:ND2	2.31	0.42
1:D:302:LEU:N	1:D:302:LEU:HD22	2.34	0.42
1:C:203:TYR:HB3	1:C:388:TYR:CD1	2.55	0.42
1:C:35:ARG:HG3	1:C:50:ARG:HH11	1.84	0.42
1:A:284:GLU:HB2	1:A:326:VAL:HG12	2.01	0.42
1:E:194:GLN:NE2	1:F:368:LEU:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLN:HE21	1:A:364:GLN:H	1.57	0.41
1:F:239:LEU:HD13	1:F:389:PHE:CE1	2.55	0.41
1:B:6:ASP:HB2	1:B:12:TYR:CE1	2.55	0.41
1:E:205:SER:HA	1:E:209:THR:HG21	2.02	0.41
1:B:35:ARG:NE	2:B:425:HOH:O	2.50	0.41
1:D:288:ILE:HG21	1:D:302:LEU:CD1	2.48	0.41
1:A:248:ASP:OD2	1:A:343:GLU:HB2	2.20	0.41
1:A:278:GLU:HG2	1:A:279:GLY:N	2.35	0.41
1:B:193:GLU:O	1:B:197:GLN:HG2	2.20	0.41
1:E:83:THR:HG21	1:E:110:TYR:CE2	2.54	0.41
1:B:87:ASN:ND2	1:B:88:ASP:N	2.65	0.41
1:A:53:GLN:HE22	1:A:314:ASP:CB	2.33	0.41
1:C:89:ASP:CG	1:C:90:ARG:N	2.73	0.41
1:D:368:LEU:HD21	1:F:190:LEU:HA	2.02	0.41
1:D:223:ASN:ND2	1:D:223:ASN:N	2.68	0.41
1:C:77:SER:OG	1:C:121:LYS:HB3	2.19	0.41
1:D:212:SER:O	1:D:242:PRO:HG2	2.20	0.41
1:E:263:LEU:HD21	1:E:390:VAL:HG11	2.03	0.41
1:C:122:MET:HB2	1:C:122:MET:HE3	1.89	0.41
1:F:72:LEU:HB3	1:F:125:LEU:HB3	2.02	0.41
1:B:23:PHE:HA	2:B:452:HOH:O	2.18	0.41
1:A:171:ARG:O	1:A:181:ARG:NH2	2.48	0.41
1:E:285:LEU:HB3	1:E:307:TYR:HB2	2.02	0.41
1:A:89:ASP:HA	1:B:360:GLN:NE2	2.35	0.41
1:F:212:GLU:HA	1:F:228:LEU:O	2.21	0.41
1:E:281:ALA:HB2	1:E:333:LEU:HD22	2.02	0.41
1:E:304:VAL:HG23	1:E:304:VAL:O	2.20	0.41
1:C:359:ARG:HB3	1:C:359:ARG:NH1	2.35	0.41
1:A:364:GLN:NE2	1:A:364:GLN:N	2.54	0.41
1:E:219:LEU:CB	1:E:236:ILE:HG12	2.50	0.41
1:D:391:ASP:O	1:F:160:THR:CG2	2.69	0.41
1:F:214:THR:HB	1:F:215:PRO:CD	2.51	0.41
1:F:239:LEU:O	1:F:326:VAL:HG23	2.21	0.41
1:C:194:PHE:CD1	1:C:194:PHE:N	2.88	0.41
1:D:101:GLN:OE1	1:D:216:PRO:HD3	2.20	0.41
1:E:289:LYS:N	1:E:303:GLU:O	2.44	0.41
1:E:349:PHE:O	1:E:356:ASN:HA	2.20	0.41
1:E:306:ARG:HD2	1:E:308:ARG:NH2	2.36	0.41
1:F:197:ARG:NH2	1:F:232:ASP:OD2	2.53	0.41
1:B:83:THR:HB	1:B:92:SER:OG	2.20	0.41
1:A:57:LYS:HB3	1:A:58:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:HIS:O	1:A:324:PRO:HA	2.21	0.41
1:D:151:GLN:OE1	1:D:176:GLU:OE1	2.37	0.41
1:C:260:ILE:CD1	1:C:311:LEU:HD11	2.47	0.41
1:D:363:ARG:NH1	1:D:374:ALA:HB3	2.35	0.41
1:A:59:ASN:HD22	1:A:195:ILE:CD1	2.33	0.41
1:F:246:LYS:H	1:F:345:ASN:ND2	2.16	0.41
1:B:384:GLN:HE21	1:B:386:GLU:H	1.69	0.41
1:A:141:SER:HB2	1:B:369:ALA:O	2.20	0.41
1:E:277:ASN:HB3	1:E:334:ASN:O	2.21	0.41
1:C:6:ASP:C	1:C:8:ASN:H	2.23	0.41
1:D:210:ILE:CD1	1:D:236:ILE:HD12	2.47	0.41
1:D:85:VAL:HG22	1:E:357:VAL:HG23	2.03	0.41
1:E:215:GLU:HB3	1:E:216:PRO:HD2	2.03	0.41
1:A:45:ASN:ND2	1:C:129:VAL:O	2.52	0.41
1:B:194:GLN:O	1:B:198:LEU:HG	2.20	0.41
1:D:278:GLU:HG2	1:D:279:GLY:N	2.36	0.41
1:D:279:GLY:HA3	1:D:332:ASN:O	2.21	0.41
1:D:29:ARG:HG2	1:D:30:ILE:N	2.36	0.41
1:C:102:ARG:HG2	1:C:103:ILE:N	2.35	0.41
1:C:65:HIS:HB3	1:C:139:PHE:CD2	2.55	0.41
1:B:103:ILE:O	1:B:104:PRO:C	2.57	0.41
1:C:68:ASP:OD2	1:C:135:TYR:HB2	2.20	0.41
1:E:83:THR:HA	1:E:92:SER:HA	2.03	0.41
1:C:384:GLN:HE21	1:C:386:GLU:HB2	1.79	0.41
1:C:32:LEU:CD2	1:C:52:VAL:HG22	2.43	0.41
1:E:220:ARG:C	1:E:222:ARG:N	2.74	0.41
1:C:174:PHE:N	1:C:174:PHE:CD2	2.87	0.41
1:D:207:ARG:NH1	1:D:207:ARG:CG	2.82	0.41
1:F:382:LYS:HD2	1:F:382:LYS:HA	1.89	0.41
1:C:102:ARG:HB3	1:C:220:GLN:HE21	1.85	0.41
1:F:195:ASN:HD22	1:F:198:SER:HB2	1.86	0.41
1:A:210:ILE:CD1	1:A:236:ILE:HD12	2.51	0.41
1:A:363:ARG:NH2	1:A:374:ALA:HB1	2.36	0.41
1:E:238:PRO:HG3	1:E:249:ILE:O	2.21	0.41
1:C:380:LEU:HD23	1:C:380:LEU:C	2.40	0.41
1:E:82:LEU:O	1:E:93:TYR:N	2.49	0.41
1:D:61:ILE:O	1:D:61:ILE:HG23	2.21	0.41
1:C:37:ASN:H	1:C:37:ASN:HD22	1.69	0.41
1:E:83:THR:HA	1:E:91:ASP:O	2.20	0.41
1:D:261:LEU:HD23	1:D:390:VAL:O	2.20	0.41
1:B:90:ARG:NH2	1:B:201:ARG:NH1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ARG:NH2	1:E:53:GLN:HE22	2.14	0.41
1:D:80:ALA:HB2	1:D:120:LEU:HD11	2.03	0.41
1:B:319:ILE:HG21	1:B:325:PHE:CD1	2.56	0.41
1:A:13:PHE:HB2	1:A:316:VAL:O	2.20	0.41
1:D:146:GLN:HB3	1:E:302:LEU:HB2	2.03	0.41
1:C:24:GLU:HG3	1:C:29:ARG:HG3	2.01	0.41
1:D:139:PHE:CE2	1:D:186:VAL:HB	2.56	0.41
1:A:380:LEU:HD21	1:C:169:ILE:HG22	2.03	0.40
1:A:68:ASP:OD2	1:A:130:ASN:ND2	2.47	0.40
1:D:213:GLU:HA	1:D:242:PRO:HG2	2.03	0.40
1:F:59:ASN:OD1	1:F:116:ASP:HA	2.20	0.40
1:E:343:GLU:O	1:E:344:ASN:HB2	2.21	0.40
1:D:171:ARG:O	1:D:181:ARG:NH2	2.54	0.40
1:E:219:LEU:HB2	1:E:236:ILE:CD1	2.51	0.40
1:F:384:GLN:HE21	1:F:386:GLU:N	2.11	0.40
1:F:384:GLN:NE2	1:F:386:GLU:CB	2.84	0.40
1:D:152:GLY:O	1:E:306:ARG:HG2	2.21	0.40
1:D:23:PHE:CE1	1:D:25:ASN:ND2	2.89	0.40
1:C:32:LEU:CD1	1:C:50:ARG:HH12	2.34	0.40
1:B:90:ARG:NH1	1:C:362:GLU:HG2	2.35	0.40
1:C:207:PHE:HB3	1:C:237:ALA:HB2	2.02	0.40
1:E:6:ASP:HB3	1:E:12:TYR:CD1	2.56	0.40
1:B:75:VAL:HA	1:B:122:MET:HG2	2.03	0.40
1:F:238:LEU:HD21	1:F:390:VAL:CG2	2.52	0.40
1:E:267:ASN:HB3	1:E:345:ASN:HD21	1.87	0.40
1:D:57:LYS:HB3	1:D:58:PRO:CD	2.50	0.40
1:D:101:GLN:HG3	1:D:102:ARG:N	2.36	0.40
1:B:321:ALA:O	1:B:322:ALA:HB3	2.20	0.40
1:C:25:ASN:C	1:C:25:ASN:OD1	2.59	0.40
1:F:196:LEU:HD23	1:F:230:SER:HB2	2.04	0.40
1:C:306:ARG:HH11	1:C:306:ARG:HG3	1.87	0.40
1:F:258:ALA:CB	1:F:333:LEU:HD22	2.49	0.40
1:E:9:ASN:C	1:E:9:ASN:ND2	2.73	0.40
1:C:190:LEU:O	1:C:190:LEU:CD2	2.69	0.40
1:A:40:SER:C	1:A:42:GLN:H	2.25	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	373/416 (90%)	348 (93%)	21 (6%)	4 (1%)	17	31
1	B	364/416 (88%)	343 (94%)	14 (4%)	7 (2%)	10	16
1	C	338/416 (81%)	306 (90%)	25 (7%)	7 (2%)	9	14
1	D	373/416 (90%)	342 (92%)	27 (7%)	4 (1%)	17	31
1	E	364/416 (88%)	340 (93%)	20 (6%)	4 (1%)	17	31
1	F	338/416 (81%)	295 (87%)	37 (11%)	6 (2%)	11	18
All	All	2150/2496 (86%)	1974 (92%)	144 (7%)	32 (2%)	13	22

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	ASP
1	C	7	GLU
1	D	6	ASP
1	E	6	ASP
1	E	201	ARG
1	F	7	GLU
1	F	331	SER
1	A	6	ASP
1	A	39	ARG
1	A	372	GLY
1	B	7	GLU
1	B	185	GLY
1	B	207	ARG
1	C	16	SER
1	C	184	GLU
1	B	388	TYR
1	D	39	ARG
1	D	372	GLY
1	F	206	ASN
1	B	229	ASN

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Mol	Chain	Res	Type
1	B	332	ASN
1	C	331	SER
1	F	15	SER
1	F	381	LEU
1	A	68	ASP
1	C	10	PRO
1	C	88	ASP
1	C	141	SER
1	D	68	ASP
1	E	39	ARG
1	E	388	TYR
1	F	10	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	341/375 (91%)	309 (91%)	32 (9%)	11	20
1	B	334/375 (89%)	301 (90%)	33 (10%)	10	18
1	C	311/375 (83%)	287 (92%)	24 (8%)	16	30
1	D	341/375 (91%)	304 (89%)	37 (11%)	8	15
1	E	334/375 (89%)	307 (92%)	27 (8%)	15	27
1	F	311/375 (83%)	287 (92%)	24 (8%)	16	30
All	All	1972/2250 (88%)	1795 (91%)	177 (9%)	12	22

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	ASN
1	A	21	THR
1	A	22	LEU
1	A	26	GLN
1	A	32	LEU

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Mol	Chain	Res	Type
1	A	37	ASN
1	A	38	LYS
1	A	39	ARG
1	A	53	GLN
1	A	62	LEU
1	A	85	VAL
1	A	87	ASN
1	A	94	ASN
1	A	102	ARG
1	A	140	LEU
1	A	142	SER
1	A	146	GLN
1	A	151	GLN
1	A	160	THR
1	A	170	ASN
1	A	207	ARG
1	A	244	LEU
1	A	250	PHE
1	A	252	SER
1	A	274	LEU
1	A	275	VAL
1	A	278	GLU
1	A	285	LEU
1	A	318	VAL
1	A	359	ARG
1	A	364	GLN
1	B	8	ASN
1	B	9	ASN
1	B	20	GLN
1	B	22	LEU
1	B	26	GLN
1	B	37	ASN
1	B	39	ARG
1	B	50	ARG
1	B	53	GLN
1	B	62	LEU
1	B	83	THR
1	B	87	ASN
1	B	94	ASN
1	B	131	LYS
1	B	140	LEU
1	B	146	GLN

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Mol	Chain	Res	Type
1	B	167	GLU
1	B	190	LEU
1	B	201	ARG
1	B	207	ARG
1	B	218	ASN
1	B	244	LEU
1	B	250	PHE
1	B	254	VAL
1	B	257	ASN
1	B	274	LEU
1	B	277	ASN
1	B	286	VAL
1	B	318	VAL
1	B	328	ASN
1	B	346	GLN
1	B	359	ARG
1	B	380	LEU
1	C	8	ASN
1	C	9	ASN
1	C	25	ASN
1	C	39	ARG
1	C	40	SER
1	C	50	ARG
1	C	53	GLN
1	C	62	LEU
1	C	87	ASN
1	C	94	ASN
1	C	113	ASN
1	C	146	GLN
1	C	170	ASN
1	C	199	ARG
1	C	227	PHE
1	C	231	VAL
1	C	251	LEU
1	C	254	ASN
1	C	257	ASP
1	C	262	LEU
1	C	308	ARG
1	C	328	ASN
1	C	368	LEU
1	C	386	GLU
1	D	8	ASN

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Mol	Chain	Res	Type
1	D	9	ASN
1	D	17	ASN
1	D	20	GLN
1	D	21	THR
1	D	22	LEU
1	D	26	GLN
1	D	32	LEU
1	D	37	ASN
1	D	38	LYS
1	D	53	GLN
1	D	62	LEU
1	D	85	VAL
1	D	87	ASN
1	D	94	ASN
1	D	95	LEU
1	D	140	LEU
1	D	146	GLN
1	D	151	GLN
1	D	157	ILE
1	D	170	ASN
1	D	176	GLU
1	D	200	ARG
1	D	221	SER
1	D	244	LEU
1	D	250	PHE
1	D	254	VAL
1	D	258	GLU
1	D	261	LEU
1	D	274	LEU
1	D	275	VAL
1	D	285	LEU
1	D	318	VAL
1	D	328	ASN
1	D	356	ASN
1	D	380	LEU
1	D	385	ARG
1	E	6	ASP
1	E	8	ASN
1	E	9	ASN
1	E	20	GLN
1	E	22	LEU
1	E	26	GLN

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Mol	Chain	Res	Type
1	E	37	ASN
1	E	62	LEU
1	E	83	THR
1	E	87	ASN
1	E	140	LEU
1	E	146	GLN
1	E	190	LEU
1	E	197	GLN
1	E	207	ARG
1	E	209	THR
1	E	218	ASN
1	E	244	LEU
1	E	250	PHE
1	E	254	VAL
1	E	274	LEU
1	E	277	ASN
1	E	286	VAL
1	E	318	VAL
1	E	328	ASN
1	E	380	LEU
1	E	385	ARG
1	F	8	ASN
1	F	9	ASN
1	F	20	GLN
1	F	22	LEU
1	F	32	LEU
1	F	37	ASN
1	F	39	ARG
1	F	53	GLN
1	F	62	LEU
1	F	85	VAL
1	F	87	ASN
1	F	94	ASN
1	F	110	TYR
1	F	140	LEU
1	F	146	GLN
1	F	170	ASN
1	F	216	GLU
1	F	221	LEU
1	F	227	PHE
1	F	251	LEU
1	F	254	ASN

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Mol	Chain	Res	Type
1	F	308	ARG
1	F	328	ASN
1	F	386	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	ASN
1	A	20	GLN
1	A	26	GLN
1	A	27	ASN
1	A	37	ASN
1	A	53	GLN
1	A	55	GLN
1	A	59	ASN
1	A	87	ASN
1	A	94	ASN
1	A	118	GLN
1	A	119	ASN
1	A	144	GLN
1	A	151	GLN
1	A	170	ASN
1	A	182	GLN
1	A	218	ASN
1	A	223	ASN
1	A	257	ASN
1	A	277	ASN
1	A	282	ASN
1	A	328	ASN
1	A	332	ASN
1	A	334	ASN
1	A	341	ASN
1	A	344	ASN
1	A	345	ASN
1	A	348	ASN
1	A	360	GLN
1	A	364	GLN
1	A	384	GLN
1	B	8	ASN
1	B	9	ASN
1	B	26	GLN

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Mol	Chain	Res	Type
1	B	27	ASN
1	B	37	ASN
1	B	53	GLN
1	B	59	ASN
1	B	87	ASN
1	B	94	ASN
1	B	118	GLN
1	B	119	ASN
1	B	144	GLN
1	B	146	GLN
1	B	218	ASN
1	B	229	ASN
1	B	243	GLN
1	B	257	ASN
1	B	277	ASN
1	B	328	ASN
1	B	332	ASN
1	B	334	ASN
1	B	341	ASN
1	B	345	ASN
1	B	360	GLN
1	B	384	GLN
1	C	8	ASN
1	C	9	ASN
1	C	37	ASN
1	C	45	ASN
1	C	53	GLN
1	C	59	ASN
1	C	65	HIS
1	C	87	ASN
1	C	94	ASN
1	C	113	ASN
1	C	118	GLN
1	C	119	ASN
1	C	146	GLN
1	C	155	HIS
1	C	156	ASN
1	C	170	ASN
1	C	183	GLN
1	C	220	GLN
1	C	234	ASN
1	C	254	ASN

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Mol	Chain	Res	Type
1	C	259	ASN
1	C	328	ASN
1	C	332	ASN
1	C	334	ASN
1	C	341	ASN
1	C	345	ASN
1	C	348	ASN
1	C	360	GLN
1	C	384	GLN
1	D	8	ASN
1	D	9	ASN
1	D	17	ASN
1	D	20	GLN
1	D	25	ASN
1	D	26	GLN
1	D	34	GLN
1	D	37	ASN
1	D	53	GLN
1	D	59	ASN
1	D	87	ASN
1	D	94	ASN
1	D	119	ASN
1	D	144	GLN
1	D	151	GLN
1	D	170	ASN
1	D	194	GLN
1	D	218	ASN
1	D	223	ASN
1	D	243	GLN
1	D	257	ASN
1	D	277	ASN
1	D	282	ASN
1	D	305	GLN
1	D	328	ASN
1	D	332	ASN
1	D	334	ASN
1	D	341	ASN
1	D	344	ASN
1	D	345	ASN
1	D	348	ASN
1	D	356	ASN
1	D	360	GLN

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Mol	Chain	Res	Type
1	D	384	GLN
1	E	8	ASN
1	E	9	ASN
1	E	26	GLN
1	E	27	ASN
1	E	34	GLN
1	E	37	ASN
1	E	45	ASN
1	E	53	GLN
1	E	59	ASN
1	E	87	ASN
1	E	94	ASN
1	E	115	HIS
1	E	118	GLN
1	E	119	ASN
1	E	144	GLN
1	E	194	GLN
1	E	218	ASN
1	E	229	ASN
1	E	243	GLN
1	E	257	ASN
1	E	277	ASN
1	E	328	ASN
1	E	332	ASN
1	E	334	ASN
1	E	341	ASN
1	E	345	ASN
1	E	346	GLN
1	E	360	GLN
1	E	384	GLN
1	F	8	ASN
1	F	9	ASN
1	F	34	GLN
1	F	37	ASN
1	F	45	ASN
1	F	53	GLN
1	F	87	ASN
1	F	94	ASN
1	F	118	GLN
1	F	119	ASN
1	F	146	GLN
1	F	147	GLN

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Mol	Chain	Res	Type
1	F	156	ASN
1	F	170	ASN
1	F	195	ASN
1	F	220	GLN
1	F	234	ASN
1	F	242	HIS
1	F	254	ASN
1	F	328	ASN
1	F	332	ASN
1	F	334	ASN
1	F	341	ASN
1	F	345	ASN
1	F	348	ASN
1	F	384	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	377/416 (90%)	-0.11	7 (1%) 70 73	18, 34, 67, 82	0
1	B	370/416 (88%)	0.03	12 (3%) 51 56	14, 36, 62, 76	0
1	C	346/416 (83%)	0.45	23 (6%) 22 24	25, 54, 74, 85	0
1	D	377/416 (90%)	-0.09	9 (2%) 62 66	17, 32, 67, 80	0
1	E	370/416 (88%)	0.09	14 (3%) 44 49	15, 39, 69, 78	0
1	F	346/416 (83%)	0.42	22 (6%) 23 25	28, 53, 75, 84	0
All	All	2186/2496 (87%)	0.12	87 (3%) 42 47	14, 40, 70, 85	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	117	HIS	5.5
1	F	301	PRO	4.7
1	C	26	GLN	4.7
1	E	207	ARG	4.4
1	D	200	ARG	4.2
1	C	301	PRO	4.2
1	E	303	GLU	3.9
1	E	117	HIS	3.7
1	C	118	GLN	3.4
1	C	23	PHE	3.4
1	C	391	ASP	3.4
1	B	145	ALA	3.4
1	E	196	ARG	3.4
1	D	196	ARG	3.3
1	B	8	ASN	3.3
1	F	26	GLN	3.3
1	E	200	ARG	3.3
1	F	199	ARG	3.2
1	D	364	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	207	ARG	3.2
1	D	289	LYS	3.2
1	E	302	LEU	3.1
1	F	392	ALA	3.1
1	A	196	ARG	3.1
1	E	208	LYS	3.1
1	A	200	ARG	3.1
1	D	201	ARG	3.0
1	A	201	ARG	3.0
1	B	184	GLU	3.0
1	F	23	PHE	3.0
1	B	385	ARG	3.0
1	A	289	LYS	2.9
1	E	171	ARG	2.9
1	F	190	LEU	2.9
1	F	198	SER	2.9
1	C	114	PRO	2.8
1	F	391	ASP	2.8
1	F	255	GLU	2.8
1	D	375	GLN	2.8
1	F	167	GLU	2.8
1	F	183	GLN	2.7
1	B	155	HIS	2.6
1	F	171	ARG	2.6
1	C	192	GLU	2.6
1	C	207	PHE	2.6
1	B	16	SER	2.6
1	E	165	GLU	2.6
1	F	302	LEU	2.5
1	E	145	ALA	2.5
1	F	200	ASN	2.5
1	E	167	GLU	2.5
1	E	193	GLU	2.4
1	C	392	ALA	2.4
1	C	115	HIS	2.4
1	F	240	LEU	2.4
1	C	17	ASN	2.4
1	A	364	GLN	2.4
1	A	303	GLU	2.4
1	C	189	GLU	2.4
1	C	385	ARG	2.3
1	C	379	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	316	VAL	2.3
1	B	239	GLU	2.3
1	D	193	GLU	2.3
1	B	206	SER	2.3
1	A	8	ASN	2.3
1	F	386	GLU	2.2
1	E	226	TYR	2.2
1	C	305	GLN	2.2
1	C	39	ARG	2.1
1	F	79	ARG	2.1
1	F	111	LEU	2.1
1	F	236	GLY	2.1
1	C	91	ASP	2.1
1	E	140	LEU	2.1
1	B	209	THR	2.1
1	B	117	HIS	2.1
1	F	117	HIS	2.1
1	D	192	LYS	2.1
1	F	20	GLN	2.0
1	D	363	ARG	2.0
1	F	385	ARG	2.0
1	C	193	PRO	2.0
1	C	167	GLU	2.0
1	C	206	ASN	2.0
1	C	390	VAL	2.0
1	B	141	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.