



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:35 am GMT

PDB ID : 2GP1
Title : Bacteriophage HK97 Prohead II crystal structure
Authors : Gertsman, I.; Gan, L.; Johnson, J.E.
Deposited on : 2006-04-15
Resolution : 5.20 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

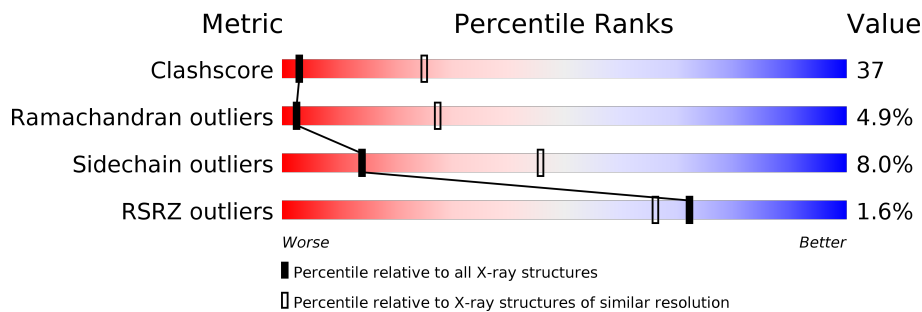
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.20 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))
Clashscore	112137	1119 (6.70-3.70)
Ramachandran outliers	110173	1051 (6.70-3.70)
Sidechain outliers	110143	1026 (6.70-3.70)
RSRZ outliers	101464	1028 (6.70-3.70)

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	282	<div> <div>43%</div> <div>37%</div> <div>9%</div> <div>•</div> <div>10%</div> </div>
1	B	282	<div>2%</div> <div>52%</div> <div>33%</div> <div>• •</div> <div>10%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13797 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 Major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1971	1233	345	383	10			
1	B	254	Total	C	N	O	S	0	0	0
			1971	1233	345	383	10			
1	C	254	Total	C	N	O	S	0	0	0
			1971	1233	345	383	10			
1	D	254	Total	C	N	O	S	0	0	0
			1971	1233	345	383	10			
1	E	254	Total	C	N	O	S	0	0	0
			1971	1233	345	383	10			
1	F	254	Total	C	N	O	S	0	0	0
			1971	1233	345	383	10			
1	G	254	Total	C	N	O	S	0	0	0
			1971	1233	345	383	10			

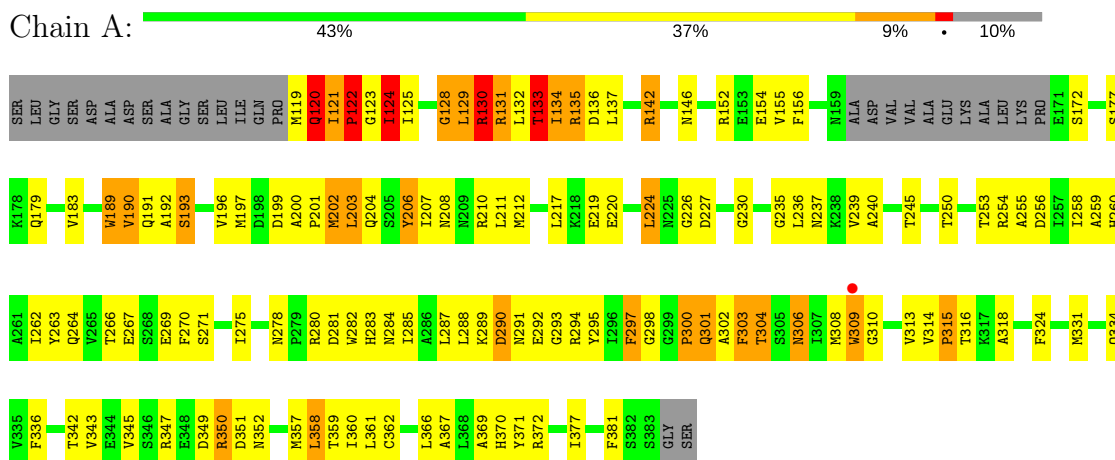
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	PHE	TRP	ENGINEERED	UNP P49861
B	336	PHE	TRP	ENGINEERED	UNP P49861
C	336	PHE	TRP	ENGINEERED	UNP P49861
D	336	PHE	TRP	ENGINEERED	UNP P49861
E	336	PHE	TRP	ENGINEERED	UNP P49861
F	336	PHE	TRP	ENGINEERED	UNP P49861
G	336	PHE	TRP	ENGINEERED	UNP P49861

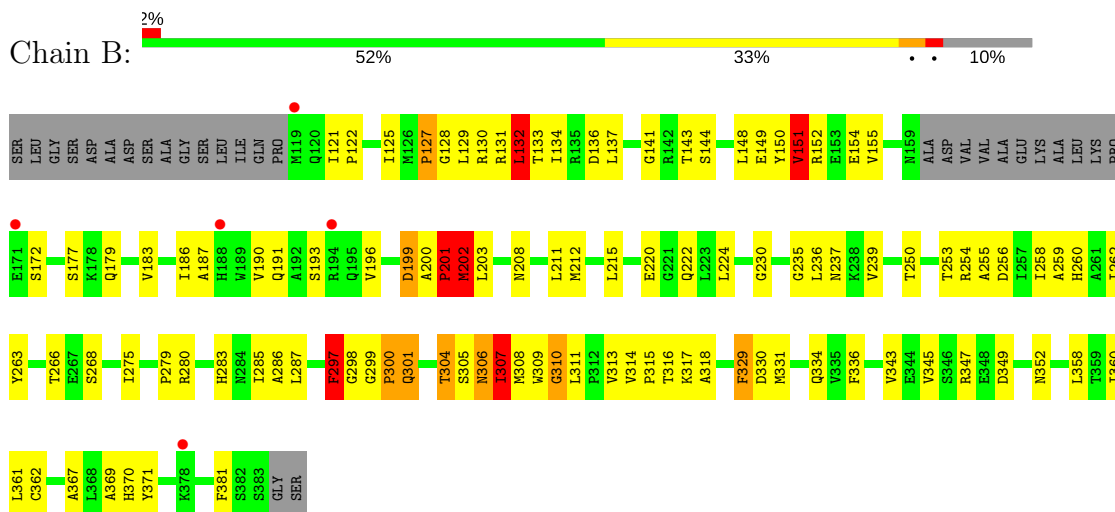
3 Residue-property plots

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

• Molecule 1: Major capsid protein

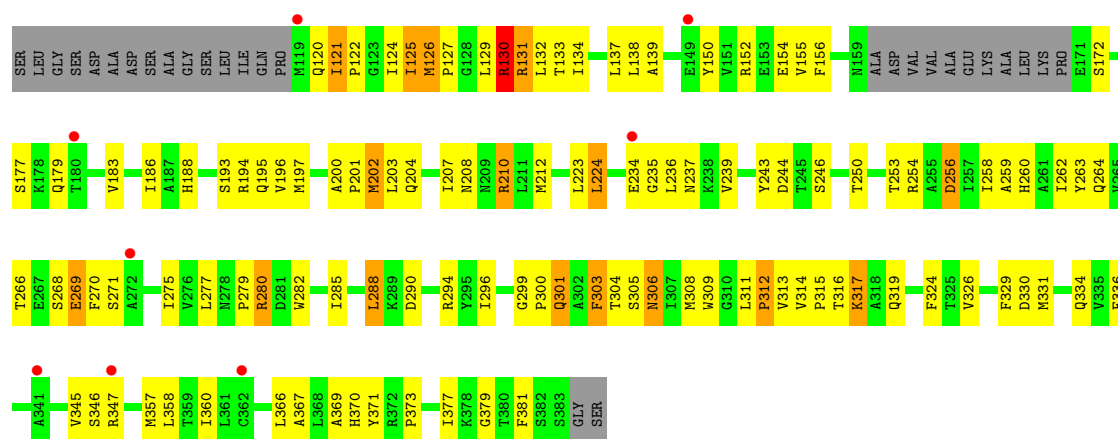


• Molecule 1: Major capsid protein

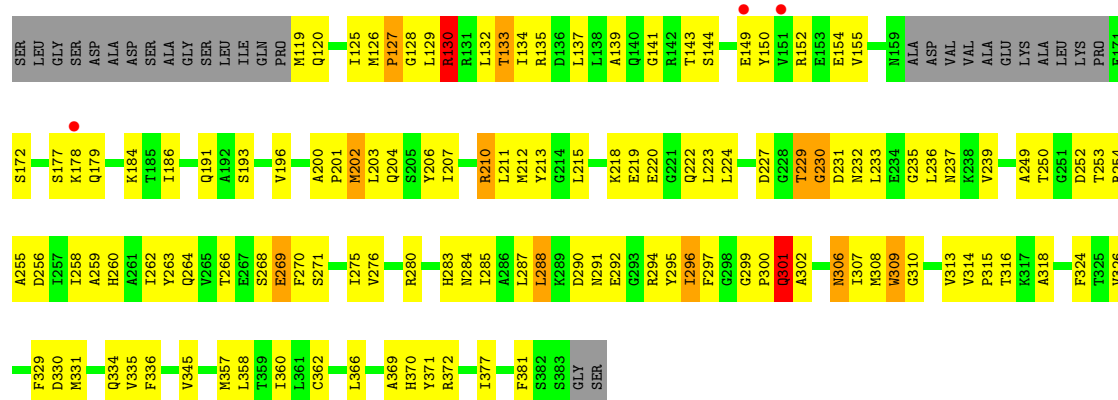
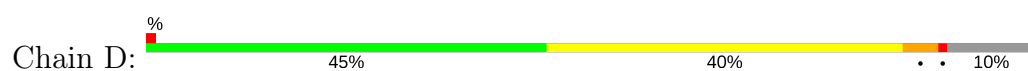


• Molecule 1: Major capsid protein

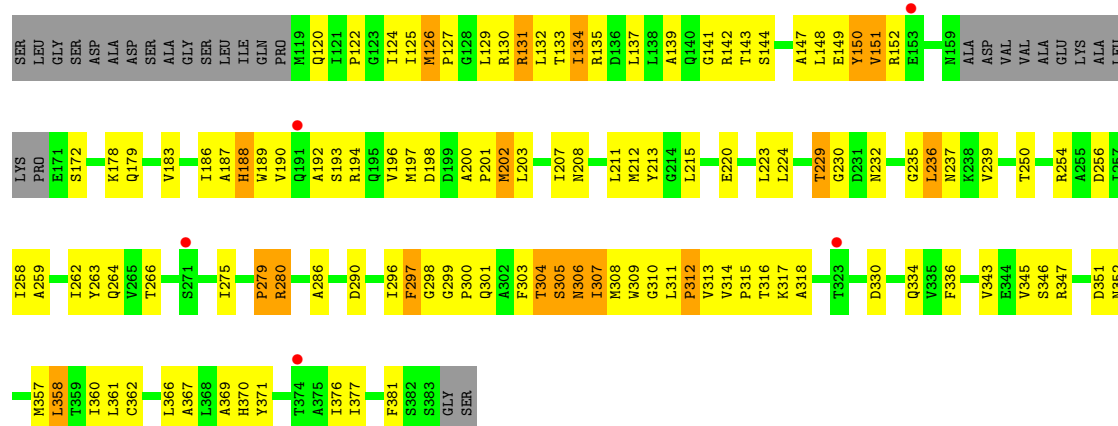




• Molecule 1: Major capsid protein

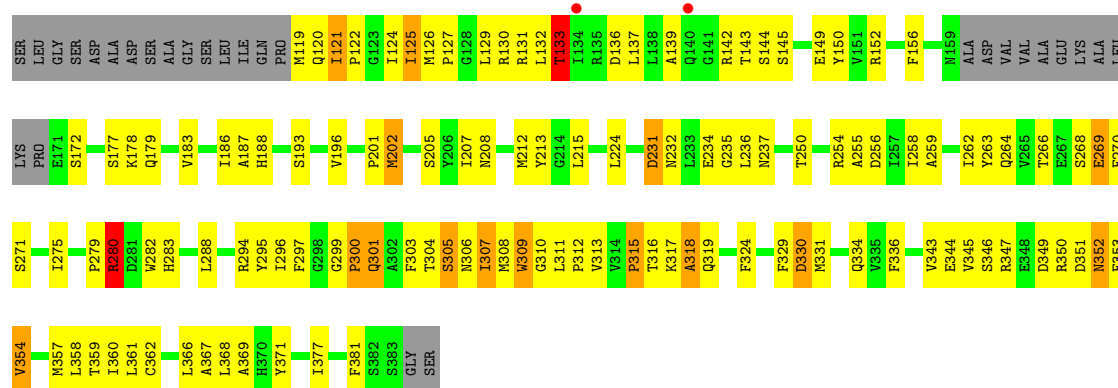


• Molecule 1: Major capsid protein

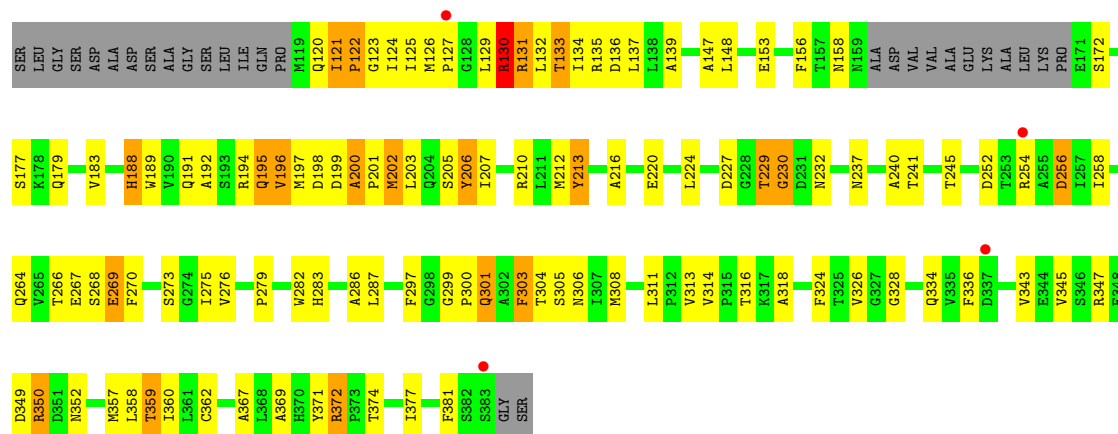


• Molecule 1: Major capsid protein





• Molecule 1: Major capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	706.94Å 706.94Å 706.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 5.20 29.98 – 5.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-5.20) 84.2 (29.98-5.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 5.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.410 , (Not available) 0.394 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	124.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 125.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.076 for l,-k,h	Xtriage
F_o, F_c correlation	0.43	EDS
Total number of atoms	13797	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.55	4/2004 (0.2%)	0.79	6/2715 (0.2%)
1	B	0.35	0/2004	0.64	1/2715 (0.0%)
1	C	0.35	0/2004	0.62	0/2715
1	D	0.36	0/2004	0.63	0/2715
1	E	0.36	0/2004	0.61	0/2715
1	F	0.61	2/2004 (0.1%)	0.68	3/2715 (0.1%)
1	G	0.36	0/2004	0.65	0/2715
All	All	0.43	6/14028 (0.0%)	0.66	10/19005 (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	G	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	231	ASP	C-N	-21.67	0.84	1.34
1	A	133	THR	N-CA	-7.60	1.31	1.46
1	A	120	GLN	C-N	7.04	1.50	1.34
1	F	280	ARG	N-CA	6.11	1.58	1.46
1	A	128	GLY	N-CA	-5.95	1.37	1.46
1	A	132	LEU	C-N	-5.75	1.20	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	PRO	CA-N-CD	-9.37	98.38	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	LEU	C-N-CA	-7.34	103.36	121.70
1	A	123	GLY	C-N-CA	7.03	139.26	121.70
1	F	318	ALA	N-CA-C	-5.91	95.04	111.00
1	A	133	THR	CA-C-N	-5.89	104.25	117.20
1	A	123	GLY	CA-C-N	-5.83	104.39	117.20
1	A	121	ILE	CB-CA-C	-5.82	99.95	111.60
1	B	202	MET	N-CA-C	5.75	126.51	111.00
1	F	133	THR	N-CA-C	5.67	126.31	111.00
1	F	280	ARG	N-CA-CB	-5.26	101.12	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	TYR	Sidechain
1	G	213	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1971	0	1937	219	0
1	B	1971	0	1938	138	0
1	C	1971	0	1938	176	0
1	D	1971	0	1937	185	0
1	E	1971	0	1938	202	0
1	F	1971	0	1936	192	0
1	G	1971	0	1938	124	0
All	All	13797	0	13562	1022	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 37.

All (1022) 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:A:280:ARG:HH22	1:B:262:ILE:CD1	1.21	1.53
1:A:280:ARG:NH2	1:B:262:ILE:HD13	1.37	1.40
1:E:279:PRO:CB	1:F:266:THR:HG21	1.51	1.39
1:A:280:ARG:NH2	1:B:262:ILE:CD1	1.88	1.36
1:C:279:PRO:CB	1:D:266:THR:HG21	1.55	1.35
1:A:134:ILE:O	1:A:136:ASP:N	1.65	1.29
1:D:202:MET:SD	1:E:143:THR:HA	1.71	1.29
1:A:266:THR:HG21	1:F:279:PRO:CB	1.67	1.25
1:F:231:ASP:C	1:F:232:ASN:CA	2.06	1.23
1:D:280:ARG:NH2	1:E:262:ILE:CD1	2.03	1.20
1:E:279:PRO:HB2	1:F:266:THR:CG2	1.74	1.18
1:F:231:ASP:O	1:F:232:ASN:N	1.77	1.18
1:B:306:ASN:HB2	1:B:313:VAL:HB	1.27	1.14
1:A:120:GLN:HG2	1:A:120:GLN:O	1.47	1.14
1:A:266:THR:HG21	1:F:279:PRO:CG	1.78	1.13
1:B:279:PRO:HB2	1:C:266:THR:HG21	1.21	1.13
1:F:231:ASP:CA	1:F:232:ASN:N	2.11	1.12
1:C:279:PRO:HB2	1:D:266:THR:HG21	1.30	1.12
1:A:134:ILE:HG22	1:A:135:ARG:N	1.64	1.11
1:E:306:ASN:HB2	1:E:313:VAL:HB	1.20	1.09
1:A:134:ILE:CG2	1:A:135:ARG:H	1.62	1.09
1:E:275:ILE:HB	1:E:313:VAL:HG22	1.34	1.08
1:D:306:ASN:HB2	1:D:313:VAL:HB	1.34	1.06
1:D:280:ARG:HH22	1:E:262:ILE:CD1	1.65	1.05
1:C:306:ASN:HB2	1:C:313:VAL:HB	1.39	1.03
1:B:275:ILE:HB	1:B:313:VAL:HG22	1.41	1.03
1:A:121:ILE:HG22	1:A:121:ILE:O	1.26	1.02
1:D:280:ARG:HA	1:E:310:GLY:HA3	1.41	1.02
1:A:280:ARG:HA	1:B:310:GLY:HA3	1.38	1.01
1:A:121:ILE:CG2	1:A:121:ILE:O	2.03	1.00
1:A:266:THR:CG2	1:F:279:PRO:HG2	1.92	1.00
1:E:336:PHE:HE1	1:E:369:ALA:HB2	1.22	1.00
1:E:197:MET:HG3	1:E:358:LEU:HD22	1.43	0.99
1:C:279:PRO:HG2	1:C:317:LYS:HB3	1.41	0.99
1:A:292:GLU:HA	1:C:294:ARG:HD2	1.40	0.98
1:A:129:LEU:O	1:A:130:ARG:HD3	1.63	0.98
1:E:196:VAL:HG22	1:F:149:GLU:HB3	1.45	0.98
1:A:280:ARG:HH22	1:B:262:ILE:HD11	1.28	0.97
1:D:280:ARG:HH22	1:E:262:ILE:HD12	1.29	0.96
1:D:280:ARG:NH2	1:E:262:ILE:HD13	1.79	0.96
1:E:279:PRO:CB	1:F:266:THR:CG2	2.37	0.96
1:A:134:ILE:HG22	1:A:135:ARG:H	0.79	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:CG2	1:A:212:MET:HG3	1.96	0.95
1:B:279:PRO:CB	1:C:266:THR:HG21	1.96	0.95
1:F:201:PRO:HG2	1:F:202:MET:SD	2.06	0.95
1:D:206:TYR:CE1	1:E:141:GLY:HA3	2.02	0.95
1:F:345:VAL:HG22	1:F:360:ILE:HG23	1.46	0.94
1:A:266:THR:HG21	1:F:279:PRO:HG2	1.45	0.94
1:A:129:LEU:HD13	1:A:130:ARG:H	1.31	0.93
1:D:206:TYR:OH	1:E:336:PHE:CE2	2.21	0.92
1:E:131:ARG:HH22	1:E:317:LYS:HG2	1.31	0.92
1:D:206:TYR:CZ	1:E:336:PHE:CE2	2.58	0.92
1:C:279:PRO:CG	1:D:266:THR:HG21	2.01	0.91
1:G:286:ALA:HA	1:G:297:PHE:HZ	1.35	0.91
1:A:125:ILE:HG21	1:A:212:MET:HG3	1.53	0.90
1:D:196:VAL:HG13	1:D:203:LEU:HG	1.54	0.89
1:D:290:ASP:HB3	1:D:296:ILE:HD11	1.51	0.89
1:F:231:ASP:C	1:F:232:ASN:N	0.84	0.88
1:E:336:PHE:CE1	1:E:369:ALA:HB2	2.08	0.88
1:C:280:ARG:HA	1:D:263:TYR:CE1	2.08	0.88
1:E:198:ASP:HB2	1:E:347:ARG:HH22	1.40	0.87
1:G:133:THR:CG2	1:G:314:VAL:HG13	2.05	0.87
1:C:317:LYS:HB2	1:D:269:GLU:OE2	1.74	0.87
1:D:210:ARG:HH21	1:E:139:ALA:HB2	1.39	0.87
1:E:336:PHE:HE1	1:E:369:ALA:CB	1.87	0.87
1:A:289:LYS:HA	1:A:295:TYR:HA	1.56	0.86
1:D:292:GLU:HA	1:F:294:ARG:HD2	1.57	0.86
1:F:119:MET:SD	1:F:344:GLU:HA	2.15	0.86
1:F:258:ILE:HB	1:F:309:TRP:CH2	2.09	0.86
1:G:224:LEU:HG	1:G:237:ASN:ND2	1.89	0.85
1:E:196:VAL:HG23	1:F:178:LYS:HZ1	1.41	0.85
1:E:317:LYS:NZ	1:F:266:THR:HA	1.92	0.85
1:C:317:LYS:HD2	1:D:269:GLU:HA	1.58	0.85
1:A:122:PRO:HB3	1:A:208:ASN:OD1	1.77	0.85
1:A:347:ARG:HG2	1:A:358:LEU:HG	1.57	0.85
1:C:280:ARG:CA	1:D:263:TYR:CE1	2.54	0.84
1:C:279:PRO:CG	1:C:317:LYS:HB3	2.06	0.84
1:D:206:TYR:OH	1:E:336:PHE:CD2	2.29	0.84
1:E:317:LYS:HB3	1:F:269:GLU:HG3	1.57	0.84
1:F:231:ASP:O	1:F:232:ASN:CA	2.21	0.84
1:C:336:PHE:HZ	1:C:371:TYR:OH	1.61	0.84
1:F:279:PRO:HD2	1:F:317:LYS:HG2	1.58	0.84
1:E:196:VAL:HG23	1:F:178:LYS:NZ	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:ILE:HB	1:F:309:TRP:HH2	1.42	0.84
1:F:119:MET:HE3	1:F:345:VAL:HG23	1.60	0.83
1:G:199:ASP:O	1:G:201:PRO:HD3	1.78	0.83
1:A:134:ILE:CD1	1:A:220:GLU:OE2	2.27	0.83
1:C:133:THR:HG21	1:C:316:THR:OG1	1.79	0.83
1:F:119:MET:SD	1:F:121:ILE:HG12	2.19	0.83
1:D:202:MET:SD	1:E:143:THR:CA	2.64	0.82
1:A:133:THR:HG21	1:A:314:VAL:HG13	1.59	0.82
1:A:266:THR:HG21	1:F:279:PRO:HB3	1.60	0.82
1:C:121:ILE:HB	1:C:122:PRO:HD3	1.58	0.82
1:F:275:ILE:HB	1:F:313:VAL:HG12	1.61	0.82
1:C:279:PRO:HB3	1:D:266:THR:HG21	1.60	0.82
1:E:275:ILE:HD12	1:E:308:MET:HB3	1.62	0.82
1:A:134:ILE:O	1:A:137:LEU:N	2.13	0.81
1:C:317:LYS:HD3	1:D:266:THR:HG23	1.62	0.81
1:B:304:THR:HG23	1:B:305:SER:H	1.46	0.81
1:A:280:ARG:HG2	1:B:310:GLY:CA	2.11	0.81
1:D:210:ARG:HH21	1:E:139:ALA:CB	1.94	0.81
1:C:201:PRO:HG2	1:C:202:MET:SD	2.22	0.80
1:G:133:THR:HG23	1:G:314:VAL:HG13	1.61	0.80
1:A:336:PHE:HE1	1:A:369:ALA:HB3	1.46	0.80
1:E:317:LYS:HZ2	1:F:270:PHE:N	1.79	0.80
1:A:131:ARG:HB3	1:A:304:THR:HG21	1.64	0.80
1:A:190:VAL:HB	1:A:211:LEU:HD21	1.63	0.80
1:A:134:ILE:HD12	1:A:220:GLU:OE2	1.82	0.80
1:A:120:GLN:O	1:A:120:GLN:CG	2.28	0.79
1:F:305:SER:HB2	1:F:315:PRO:HD3	1.64	0.79
1:F:336:PHE:HZ	1:F:371:TYR:OH	1.65	0.79
1:C:306:ASN:HD21	1:C:315:PRO:HD3	1.47	0.79
1:A:280:ARG:HH22	1:B:262:ILE:HD12	1.38	0.79
1:F:133:THR:HG22	1:F:136:ASP:HB2	1.64	0.79
1:D:202:MET:SD	1:D:203:LEU:N	2.55	0.79
1:A:122:PRO:HG2	1:A:343:VAL:O	1.82	0.79
1:D:280:ARG:HG2	1:E:310:GLY:C	2.03	0.79
1:B:128:GLY:HA3	1:B:131:ARG:HB2	1.63	0.78
1:C:279:PRO:HG2	1:C:317:LYS:CB	2.13	0.78
1:A:124:ILE:O	1:A:125:ILE:HD13	1.83	0.78
1:B:300:PRO:HA	1:C:309:TRP:CZ3	2.17	0.78
1:B:317:LYS:NZ	1:C:266:THR:HA	1.98	0.78
1:A:129:LEU:CD1	1:A:130:ARG:H	1.96	0.77
1:E:317:LYS:HZ3	1:F:266:THR:HA	1.45	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HD22	1:B:362:CYS:SG	2.25	0.77
1:B:187:ALA:HB1	1:B:361:LEU:HD11	1.65	0.77
1:G:203:LEU:HA	1:G:206:TYR:HB3	1.67	0.76
1:G:203:LEU:HG	1:G:206:TYR:HD2	1.48	0.76
1:C:279:PRO:HG2	1:D:266:THR:CG2	2.14	0.76
1:D:280:ARG:HG2	1:E:310:GLY:CA	2.15	0.76
1:G:229:THR:CG2	1:G:232:ASN:HD22	1.98	0.76
1:G:316:THR:HG22	1:G:318:ALA:H	1.49	0.76
1:A:301:GLN:HG2	1:A:302:ALA:H	1.50	0.76
1:D:202:MET:HE1	1:E:144:SER:H	1.51	0.76
1:F:133:THR:O	1:F:137:LEU:HG	1.85	0.75
1:A:196:VAL:HG12	1:A:203:LEU:HD22	1.68	0.75
1:D:137:LEU:HD11	1:D:314:VAL:HG21	1.69	0.75
1:E:211:LEU:HD21	1:E:360:ILE:HG23	1.68	0.75
1:G:336:PHE:HZ	1:G:371:TYR:HH	1.34	0.75
1:A:336:PHE:HE1	1:A:369:ALA:CB	2.00	0.74
1:B:317:LYS:HB3	1:C:269:GLU:HG3	1.69	0.74
1:E:200:ALA:HB3	1:E:203:LEU:HB2	1.69	0.74
1:A:134:ILE:HG13	1:A:220:GLU:OE2	1.86	0.74
1:G:125:ILE:HD12	1:G:125:ILE:H	1.51	0.74
1:D:280:ARG:HH21	1:E:262:ILE:CD1	2.00	0.74
1:A:134:ILE:C	1:A:136:ASP:N	2.40	0.74
1:E:134:ILE:HD13	1:E:224:LEU:HB2	1.70	0.74
1:C:279:PRO:CB	1:D:266:THR:CG2	2.51	0.73
1:G:197:MET:SD	1:G:207:ILE:HD13	2.28	0.73
1:D:258:ILE:O	1:D:262:ILE:HG13	1.88	0.73
1:C:186:ILE:HD12	1:C:366:LEU:HD12	1.70	0.73
1:G:121:ILE:HG22	1:G:124:ILE:HG12	1.70	0.73
1:A:134:ILE:CG1	1:A:220:GLU:OE2	2.37	0.73
1:C:279:PRO:HB2	1:D:266:THR:CG2	2.15	0.73
1:G:254:ARG:HB3	1:G:381:PHE:CE2	2.24	0.73
1:A:129:LEU:C	1:A:130:ARG:HD3	2.09	0.72
1:B:183:VAL:HG22	1:B:367:ALA:HB2	1.71	0.72
1:B:215:LEU:HB2	1:B:362:CYS:SG	2.29	0.72
1:F:258:ILE:O	1:F:262:ILE:HG13	1.89	0.72
1:G:254:ARG:HB3	1:G:381:PHE:HE2	1.53	0.72
1:B:306:ASN:OD1	1:B:315:PRO:HG3	1.89	0.72
1:A:306:ASN:ND2	1:A:313:VAL:HB	2.04	0.72
1:D:280:ARG:CA	1:E:310:GLY:HA3	2.18	0.71
1:A:134:ILE:HD12	1:A:220:GLU:CD	2.11	0.71
1:A:280:ARG:NH2	1:B:262:ILE:HD11	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ILE:O	1:B:127:PRO:HD3	1.91	0.71
1:A:196:VAL:HG21	1:B:149:GLU:HB2	1.72	0.71
1:D:264:GLN:HB3	1:D:377:ILE:HD13	1.71	0.71
1:E:279:PRO:HB2	1:F:266:THR:HG21	0.77	0.71
1:A:280:ARG:HG2	1:B:310:GLY:HA3	1.71	0.71
1:C:336:PHE:HZ	1:C:371:TYR:HH	1.36	0.71
1:D:285:ILE:O	1:D:288:LEU:HB2	1.90	0.71
1:E:301:GLN:HA	1:F:309:TRP:HA	1.72	0.71
1:A:258:ILE:HG21	1:A:275:ILE:HD13	1.72	0.71
1:B:154:GLU:HG3	1:B:155:VAL:HG23	1.72	0.71
1:A:134:ILE:O	1:A:135:ARG:C	2.29	0.71
1:A:294:ARG:CZ	1:D:290:ASP:HB2	2.21	0.71
1:E:193:SER:HB3	1:F:178:LYS:NZ	2.05	0.71
1:E:286:ALA:HB1	1:E:299:GLY:H	1.56	0.71
1:F:352:ASN:HD21	1:F:359:THR:N	1.88	0.71
1:E:307:ILE:HG12	1:E:312:PRO:HA	1.73	0.71
1:G:229:THR:HG23	1:G:230:GLY:N	2.06	0.71
1:D:336:PHE:HZ	1:D:371:TYR:HH	1.39	0.70
1:E:300:PRO:O	1:F:309:TRP:HB3	1.89	0.70
1:A:191:GLN:NE2	1:A:357:MET:HB3	2.06	0.70
1:C:279:PRO:CD	1:C:317:LYS:HB3	2.21	0.70
1:F:224:LEU:HD13	1:F:237:ASN:ND2	2.06	0.70
1:A:347:ARG:H	1:A:359:THR:HB	1.56	0.70
1:A:183:VAL:HG22	1:A:367:ALA:HB2	1.74	0.70
1:D:280:ARG:HH21	1:E:262:ILE:HD13	1.56	0.70
1:G:276:VAL:HG13	1:G:314:VAL:HG12	1.72	0.70
1:E:306:ASN:ND2	1:E:315:PRO:HD3	2.07	0.70
1:E:279:PRO:HG2	1:F:266:THR:HG23	1.73	0.70
1:F:231:ASP:O	1:F:232:ASN:HA	1.92	0.70
1:A:121:ILE:N	1:A:122:PRO:HD3	2.07	0.70
1:C:244:ASP:OD1	1:C:246:SER:HB3	1.92	0.70
1:D:206:TYR:CZ	1:E:336:PHE:CD2	2.79	0.70
1:E:131:ARG:HD2	1:E:133:THR:HG23	1.73	0.69
1:A:280:ARG:HD3	1:B:309:TRP:HB3	1.72	0.69
1:D:275:ILE:HB	1:D:313:VAL:HG22	1.73	0.69
1:D:128:GLY:HA3	1:D:132:LEU:HD21	1.74	0.69
1:B:280:ARG:NE	1:C:263:TYR:OH	2.26	0.69
1:C:336:PHE:CZ	1:C:371:TYR:OH	2.45	0.69
1:E:131:ARG:NH2	1:E:317:LYS:HG2	2.07	0.69
1:C:279:PRO:CG	1:D:266:THR:CG2	2.71	0.69
1:F:119:MET:SD	1:F:343:VAL:O	2.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:PHE:HE1	1:G:369:ALA:CB	2.06	0.69
1:B:316:THR:HG22	1:B:318:ALA:H	1.56	0.69
1:D:280:ARG:HA	1:E:310:GLY:CA	2.20	0.69
1:A:134:ILE:HD12	1:A:220:GLU:CG	2.23	0.68
1:A:258:ILE:HD12	1:A:258:ILE:H	1.57	0.68
1:E:133:THR:HG22	1:E:314:VAL:CG1	2.23	0.68
1:E:308:MET:C	1:E:310:GLY:H	1.96	0.68
1:D:200:ALA:HB1	1:D:204:GLN:HB2	1.74	0.68
1:D:283:HIS:CE1	1:D:287:LEU:HD11	2.29	0.68
1:F:307:ILE:HG23	1:F:310:GLY:HA2	1.76	0.68
1:A:219:GLU:HG3	1:A:366:LEU:HD11	1.76	0.68
1:C:258:ILE:O	1:C:262:ILE:HG13	1.94	0.68
1:A:258:ILE:O	1:A:262:ILE:HG13	1.94	0.68
1:G:336:PHE:CE1	1:G:369:ALA:CB	2.77	0.68
1:C:130:ARG:HG3	1:D:271:SER:HB2	1.76	0.67
1:G:227:ASP:HB3	1:G:229:THR:HG22	1.77	0.67
1:A:259:ALA:HB2	1:A:309:TRP:HE1	1.59	0.67
1:B:345:VAL:HG22	1:B:360:ILE:HG23	1.76	0.67
1:E:275:ILE:O	1:E:313:VAL:HG13	1.95	0.67
1:E:279:PRO:CG	1:F:266:THR:HG21	2.21	0.67
1:A:129:LEU:HD13	1:A:130:ARG:N	2.07	0.67
1:B:134:ILE:HD12	1:B:220:GLU:HB3	1.75	0.67
1:E:130:ARG:HG3	1:E:131:ARG:HG3	1.76	0.67
1:E:347:ARG:HG2	1:E:358:LEU:HD11	1.76	0.67
1:F:336:PHE:HZ	1:F:371:TYR:HH	1.41	0.67
1:B:215:LEU:HD13	1:B:362:CYS:HB3	1.76	0.67
1:C:301:GLN:HB2	1:D:309:TRP:HA	1.77	0.67
1:G:229:THR:HG23	1:G:230:GLY:H	1.59	0.67
1:G:345:VAL:HG22	1:G:360:ILE:HG23	1.77	0.67
1:A:263:TYR:CE1	1:F:280:ARG:N	2.63	0.67
1:G:124:ILE:HD12	1:G:212:MET:HE2	1.75	0.67
1:D:202:MET:C	1:D:202:MET:SD	2.74	0.66
1:G:132:LEU:HD22	1:G:135:ARG:HB3	1.78	0.66
1:A:285:ILE:O	1:A:288:LEU:HB2	1.94	0.66
1:E:308:MET:HG3	1:E:309:TRP:HD1	1.58	0.66
1:G:192:ALA:O	1:G:358:LEU:HB2	1.95	0.66
1:A:306:ASN:HD21	1:A:313:VAL:HB	1.61	0.66
1:A:192:ALA:O	1:A:358:LEU:HD22	1.94	0.66
1:B:128:GLY:CA	1:B:131:ARG:HB2	2.26	0.66
1:E:198:ASP:HB2	1:E:347:ARG:NH2	2.07	0.66
1:E:215:LEU:HD22	1:E:362:CYS:SG	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:HD12	1:A:258:ILE:N	2.10	0.66
1:A:266:THR:HG21	1:F:279:PRO:HB2	1.75	0.66
1:C:317:LYS:HD3	1:D:266:THR:CG2	2.26	0.66
1:A:146:ASN:HD21	1:G:147:ALA:HB3	1.61	0.66
1:C:317:LYS:CD	1:D:266:THR:HG23	2.26	0.66
1:A:316:THR:HG22	1:A:318:ALA:H	1.59	0.65
1:F:187:ALA:HB1	1:F:361:LEU:HD11	1.77	0.65
1:B:152:ARG:HG2	1:B:179:GLN:HG3	1.77	0.65
1:D:283:HIS:CE1	1:E:307:ILE:HB	2.31	0.65
1:A:301:GLN:HG2	1:A:302:ALA:N	2.11	0.65
1:C:131:ARG:NE	1:C:131:ARG:HA	2.12	0.65
1:C:280:ARG:N	1:D:263:TYR:CE1	2.63	0.65
1:E:307:ILE:HG22	1:E:310:GLY:HA2	1.78	0.65
1:F:353:PHE:HD2	1:G:359:THR:HG22	1.62	0.65
1:A:134:ILE:C	1:A:136:ASP:H	2.00	0.65
1:A:260:HIS:ND1	1:F:283:HIS:NE2	2.45	0.65
1:A:202:MET:SD	1:B:143:THR:HA	2.37	0.65
1:C:306:ASN:ND2	1:C:315:PRO:HD3	2.11	0.65
1:D:133:THR:O	1:D:137:LEU:HG	1.97	0.65
1:F:183:VAL:HG22	1:F:367:ALA:HB2	1.78	0.65
1:F:119:MET:CE	1:F:345:VAL:HG23	2.26	0.65
1:C:306:ASN:HD21	1:C:315:PRO:CD	2.10	0.65
1:E:264:GLN:HB3	1:E:377:ILE:HD13	1.77	0.65
1:A:292:GLU:HG2	1:A:294:ARG:NH2	2.12	0.64
1:A:191:GLN:HE22	1:A:357:MET:HB3	1.62	0.64
1:C:130:ARG:NH2	1:C:131:ARG:HG2	2.13	0.64
1:C:154:GLU:HG3	1:C:155:VAL:HG23	1.79	0.64
1:D:345:VAL:HG22	1:D:360:ILE:HG23	1.77	0.64
1:G:131:ARG:C	1:G:133:THR:H	2.00	0.64
1:G:324:PHE:HB3	1:G:381:PHE:HE1	1.61	0.64
1:A:202:MET:SD	1:A:203:LEU:N	2.70	0.64
1:E:187:ALA:HB1	1:E:361:LEU:HD11	1.78	0.64
1:G:207:ILE:HG21	1:G:360:ILE:HD13	1.80	0.64
1:B:347:ARG:HD2	1:B:358:LEU:HD11	1.79	0.64
1:E:279:PRO:CG	1:F:266:THR:CG2	2.75	0.64
1:A:259:ALA:CB	1:A:309:TRP:HE1	2.11	0.64
1:E:197:MET:SD	1:E:207:ILE:HD13	2.38	0.64
1:A:263:TYR:CZ	1:F:280:ARG:CA	2.81	0.63
1:D:206:TYR:CE1	1:E:141:GLY:CA	2.79	0.63
1:D:276:VAL:HG22	1:D:314:VAL:HB	1.80	0.63
1:E:194:ARG:HA	1:E:358:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:ASP:O	1:G:352:ASN:HB2	1.98	0.63
1:C:183:VAL:HG22	1:C:367:ALA:HB2	1.78	0.63
1:C:125:ILE:HG22	1:C:126:MET:H	1.63	0.63
1:A:190:VAL:HG12	1:A:360:ILE:HB	1.81	0.63
1:A:280:ARG:HD3	1:B:309:TRP:CB	2.28	0.63
1:A:298:GLY:C	1:A:300:PRO:HD3	2.19	0.63
1:B:201:PRO:O	1:B:202:MET:SD	2.57	0.63
1:D:154:GLU:HG3	1:D:155:VAL:HG23	1.79	0.63
1:D:280:ARG:NH2	1:E:262:ILE:HD11	2.08	0.63
1:E:130:ARG:HG2	1:F:271:SER:HB2	1.81	0.63
1:A:324:PHE:HB3	1:A:381:PHE:HE1	1.64	0.63
1:B:301:GLN:CD	1:B:301:GLN:H	2.03	0.63
1:D:177:SER:HB2	1:D:179:GLN:HE21	1.63	0.63
1:G:188:HIS:CD2	1:G:362:CYS:HB3	2.34	0.63
1:C:275:ILE:O	1:C:313:VAL:HG13	1.99	0.62
1:E:307:ILE:HG22	1:E:310:GLY:CA	2.29	0.62
1:B:286:ALA:HB1	1:B:299:GLY:HA3	1.81	0.62
1:D:229:THR:HG23	1:D:232:ASN:HD22	1.64	0.62
1:B:317:LYS:HZ3	1:C:266:THR:HA	1.62	0.62
1:A:294:ARG:NH2	1:D:290:ASP:HB2	2.14	0.62
1:G:336:PHE:CE1	1:G:369:ALA:HB2	2.33	0.62
1:F:308:MET:HB3	1:F:313:VAL:HG11	1.81	0.62
1:B:307:ILE:HG22	1:B:310:GLY:C	2.20	0.62
1:C:317:LYS:CB	1:D:269:GLU:OE2	2.46	0.62
1:D:229:THR:HG23	1:D:230:GLY:N	2.14	0.62
1:C:133:THR:HG22	1:C:134:ILE:N	2.15	0.62
1:F:282:TRP:CZ3	1:F:308:MET:SD	2.92	0.62
1:A:280:ARG:CA	1:B:310:GLY:HA3	2.23	0.62
1:A:203:LEU:CD1	1:B:148:LEU:HD22	2.29	0.62
1:A:331:MET:HG3	1:A:372:ARG:NH2	2.14	0.62
1:F:357:MET:O	1:F:358:LEU:HD13	1.99	0.62
1:B:317:LYS:HZ2	1:C:270:PHE:N	1.97	0.62
1:D:264:GLN:HB3	1:D:377:ILE:CD1	2.29	0.62
1:G:202:MET:HG2	1:G:203:LEU:HD13	1.82	0.62
1:F:125:ILE:O	1:F:127:PRO:HD3	2.00	0.62
1:F:282:TRP:HZ3	1:F:308:MET:SD	2.22	0.62
1:G:343:VAL:HG22	1:G:362:CYS:SG	2.39	0.61
1:G:336:PHE:HZ	1:G:371:TYR:OH	1.83	0.61
1:D:294:ARG:HH11	1:F:299:GLY:HA2	1.64	0.61
1:D:207:ILE:HG21	1:D:360:ILE:HD13	1.82	0.61
1:E:130:ARG:HG2	1:F:271:SER:CB	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ILE:HD12	1:C:313:VAL:HG22	1.82	0.61
1:E:211:LEU:HD23	1:E:343:VAL:HG13	1.81	0.61
1:C:345:VAL:HG22	1:C:360:ILE:HG23	1.82	0.61
1:D:206:TYR:CE2	1:E:336:PHE:HE2	2.18	0.61
1:G:336:PHE:HB2	1:G:367:ALA:HB3	1.81	0.61
1:C:224:LEU:HD13	1:C:237:ASN:ND2	2.15	0.61
1:F:301:GLN:O	1:F:301:GLN:HG2	2.01	0.61
1:B:300:PRO:HA	1:C:309:TRP:HZ3	1.65	0.60
1:E:236:LEU:HD12	1:E:376:ILE:HD13	1.82	0.60
1:E:290:ASP:HB3	1:E:296:ILE:HD11	1.83	0.60
1:G:156:PHE:CE2	1:G:158:ASN:HB2	2.36	0.60
1:A:226:GLY:HA3	1:A:235:GLY:H	1.66	0.60
1:C:303:PHE:HZ	1:D:263:TYR:HB2	1.65	0.60
1:D:280:ARG:HG2	1:E:310:GLY:HA3	1.83	0.60
1:D:316:THR:HG22	1:D:318:ALA:H	1.66	0.60
1:A:134:ILE:HD12	1:A:220:GLU:HG2	1.82	0.60
1:A:267:GLU:HA	1:F:317:LYS:NZ	2.16	0.60
1:C:317:LYS:HZ1	1:D:270:PHE:C	2.04	0.60
1:E:258:ILE:O	1:E:262:ILE:HG13	2.00	0.60
1:G:197:MET:SD	1:G:207:ILE:CD1	2.89	0.60
1:B:150:TYR:O	1:B:151:VAL:HG13	2.00	0.60
1:C:125:ILE:HG22	1:C:126:MET:N	2.17	0.60
1:E:306:ASN:HB2	1:E:313:VAL:CB	2.13	0.60
1:G:286:ALA:HA	1:G:297:PHE:CZ	2.27	0.60
1:D:206:TYR:CE2	1:E:336:PHE:CE2	2.89	0.60
1:D:256:ASP:O	1:D:259:ALA:HB3	2.01	0.60
1:E:360:ILE:HG22	1:E:360:ILE:O	2.02	0.60
1:A:122:PRO:CG	1:A:343:VAL:O	2.50	0.59
1:A:280:ARG:HE	1:B:311:LEU:HG	1.67	0.59
1:B:224:LEU:HD13	1:B:237:ASN:HD22	1.67	0.59
1:D:134:ILE:HB	1:D:220:GLU:HG3	1.85	0.59
1:G:264:GLN:HB3	1:G:377:ILE:HD13	1.84	0.59
1:A:290:ASP:HB2	1:D:292:GLU:HG2	1.83	0.59
1:B:349:ASP:O	1:B:352:ASN:HB2	2.02	0.59
1:C:317:LYS:NZ	1:D:266:THR:HA	2.17	0.59
1:B:196:VAL:HB	1:B:203:LEU:HD22	1.83	0.59
1:D:201:PRO:HB2	1:D:202:MET:HE2	1.83	0.59
1:F:224:LEU:HD13	1:F:237:ASN:HD22	1.66	0.59
1:A:142:ARG:O	1:F:202:MET:SD	2.61	0.59
1:A:361:LEU:HG	1:A:362:CYS:H	1.67	0.59
1:C:301:GLN:C	1:C:303:PHE:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:THR:HG22	1:F:317:LYS:HG3	1.85	0.59
1:E:279:PRO:HG2	1:F:266:THR:CG2	2.31	0.59
1:B:317:LYS:HB3	1:C:269:GLU:OE2	2.03	0.59
1:C:210:ARG:HG3	1:C:210:ARG:HH11	1.66	0.59
1:E:301:GLN:HA	1:F:309:TRP:CA	2.33	0.59
1:E:131:ARG:HH22	1:E:317:LYS:CG	2.12	0.59
1:B:122:PRO:HD2	1:B:208:ASN:HD22	1.68	0.58
1:E:264:GLN:HB3	1:E:377:ILE:CD1	2.32	0.58
1:A:267:GLU:HA	1:F:317:LYS:CE	2.33	0.58
1:A:336:PHE:CE1	1:A:369:ALA:CB	2.85	0.58
1:B:279:PRO:CB	1:C:266:THR:CG2	2.79	0.58
1:C:290:ASP:HB3	1:C:296:ILE:HD11	1.85	0.58
1:B:317:LYS:HZ2	1:C:269:GLU:C	2.06	0.58
1:D:152:ARG:HB2	1:D:371:TYR:O	2.03	0.58
1:A:134:ILE:CG2	1:A:135:ARG:N	2.36	0.58
1:D:219:GLU:HG3	1:D:366:LEU:HD11	1.85	0.58
1:C:280:ARG:N	1:D:263:TYR:HE1	2.01	0.58
1:B:134:ILE:HD13	1:B:224:LEU:HB2	1.85	0.58
1:D:336:PHE:HE1	1:D:369:ALA:CB	2.17	0.58
1:E:131:ARG:HD2	1:E:133:THR:CG2	2.34	0.58
1:E:307:ILE:HG22	1:E:310:GLY:C	2.24	0.58
1:B:224:LEU:HD13	1:B:237:ASN:ND2	2.18	0.58
1:A:202:MET:HE2	1:B:144:SER:H	1.69	0.58
1:D:201:PRO:HD2	1:D:202:MET:HE3	1.84	0.58
1:G:276:VAL:HG13	1:G:314:VAL:CG1	2.33	0.58
1:E:196:VAL:HG22	1:F:149:GLU:CB	2.29	0.58
1:E:189:TRP:HA	1:E:360:ILE:O	2.05	0.57
1:G:275:ILE:O	1:G:314:VAL:HB	2.04	0.57
1:A:258:ILE:CD1	1:A:258:ILE:H	2.16	0.57
1:A:280:ARG:HH21	1:B:262:ILE:HD13	1.55	0.57
1:C:279:PRO:CD	1:C:317:LYS:HA	2.34	0.57
1:F:361:LEU:HG	1:F:362:CYS:N	2.19	0.57
1:D:133:THR:HB	1:D:314:VAL:HG13	1.86	0.57
1:D:280:ARG:CZ	1:E:309:TRP:HB2	2.35	0.57
1:F:224:LEU:O	1:F:237:ASN:HB2	2.05	0.57
1:G:282:TRP:CD2	1:G:313:VAL:HG11	2.38	0.57
1:F:255:ALA:HB1	1:F:309:TRP:HZ2	1.70	0.57
1:F:255:ALA:O	1:F:309:TRP:CH2	2.58	0.57
1:E:306:ASN:ND2	1:E:306:ASN:H	2.02	0.57
1:C:317:LYS:HZ3	1:D:266:THR:HA	1.70	0.57
1:F:300:PRO:HG2	1:F:301:GLN:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:GLN:HB3	1:C:377:ILE:HD13	1.87	0.56
1:D:280:ARG:NH1	1:E:309:TRP:HB2	2.20	0.56
1:F:352:ASN:HD21	1:F:359:THR:H	1.54	0.56
1:G:314:VAL:O	1:G:314:VAL:HG12	2.05	0.56
1:A:125:ILE:HG21	1:A:212:MET:CG	2.33	0.56
1:G:229:THR:HG22	1:G:232:ASN:HD22	1.69	0.56
1:A:254:ARG:HB3	1:A:381:PHE:HE2	1.70	0.56
1:D:193:SER:OG	1:D:196:VAL:HG23	2.06	0.56
1:A:134:ILE:O	1:A:136:ASP:CA	2.51	0.56
1:A:206:TYR:HE2	1:A:210:ARG:HD3	1.71	0.56
1:C:208:ASN:O	1:C:212:MET:HG2	2.05	0.56
1:E:317:LYS:HB3	1:F:269:GLU:CG	2.32	0.56
1:A:177:SER:HB3	1:A:179:GLN:HE21	1.71	0.56
1:D:203:LEU:O	1:D:203:LEU:HD12	2.06	0.56
1:D:294:ARG:HH11	1:F:299:GLY:CA	2.18	0.56
1:B:343:VAL:HG22	1:B:362:CYS:SG	2.46	0.56
1:G:130:ARG:NE	1:G:130:ARG:HA	2.19	0.56
1:A:199:ASP:C	1:A:201:PRO:HD3	2.26	0.56
1:A:239:VAL:HG21	1:A:370:HIS:CG	2.41	0.56
1:B:256:ASP:O	1:B:259:ALA:HB3	2.05	0.56
1:C:133:THR:HG23	1:C:314:VAL:HG11	1.86	0.56
1:G:224:LEU:HG	1:G:237:ASN:HD21	1.69	0.56
1:E:150:TYR:O	1:E:178:LYS:HA	2.07	0.55
1:A:256:ASP:O	1:A:259:ALA:HB3	2.06	0.55
1:C:279:PRO:HD3	1:C:317:LYS:HA	1.88	0.55
1:E:306:ASN:HD22	1:E:306:ASN:H	1.54	0.55
1:A:193:SER:HB3	1:A:196:VAL:HG23	1.87	0.55
1:A:352:ASN:CB	1:A:357:MET:HB2	2.36	0.55
1:B:286:ALA:HB1	1:B:299:GLY:CA	2.36	0.55
1:B:137:LEU:HD11	1:B:314:VAL:HG21	1.88	0.55
1:C:244:ASP:HB2	1:C:264:GLN:HE22	1.71	0.55
1:E:280:ARG:HA	1:F:263:TYR:CE1	2.42	0.55
1:E:336:PHE:HB2	1:E:367:ALA:HB3	1.87	0.55
1:E:317:LYS:NZ	1:F:270:PHE:N	2.54	0.55
1:G:300:PRO:O	1:G:301:GLN:HG3	2.07	0.55
1:B:127:PRO:HG2	1:B:128:GLY:H	1.71	0.55
1:C:134:ILE:O	1:C:138:LEU:HG	2.06	0.55
1:C:277:LEU:HD11	1:C:308:MET:CE	2.37	0.55
1:D:229:THR:CG2	1:D:232:ASN:HD22	2.19	0.55
1:E:211:LEU:CD2	1:E:360:ILE:HG23	2.36	0.55
1:E:305:SER:C	1:E:307:ILE:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:SER:HB3	1:F:178:LYS:HZ2	1.68	0.55
1:F:275:ILE:HB	1:F:313:VAL:CG1	2.33	0.55
1:F:349:ASP:O	1:F:352:ASN:HB2	2.06	0.55
1:G:196:VAL:HG12	1:G:203:LEU:HD22	1.88	0.55
1:B:131:ARG:HD3	1:C:271:SER:OG	2.07	0.55
1:E:124:ILE:HB	1:E:212:MET:HG3	1.89	0.55
1:E:280:ARG:NE	1:F:263:TYR:CE2	2.71	0.55
1:C:308:MET:HB3	1:C:313:VAL:HG21	1.89	0.55
1:D:262:ILE:HD12	1:D:309:TRP:CD1	2.41	0.55
1:A:266:THR:CG2	1:F:279:PRO:CG	2.56	0.55
1:G:139:ALA:HB3	1:G:334:GLN:HB3	1.88	0.55
1:A:255:ALA:HB1	1:A:309:TRP:CH2	2.42	0.55
1:D:336:PHE:HZ	1:D:371:TYR:OH	1.89	0.55
1:A:263:TYR:CE1	1:F:280:ARG:CA	2.90	0.55
1:A:308:MET:O	1:A:309:TRP:HB2	2.06	0.55
1:C:275:ILE:HB	1:C:313:VAL:HG22	1.87	0.55
1:C:279:PRO:HG2	1:C:317:LYS:CG	2.37	0.55
1:E:300:PRO:C	1:F:309:TRP:HB3	2.26	0.55
1:F:307:ILE:HG23	1:F:310:GLY:CA	2.37	0.55
1:A:146:ASN:ND2	1:G:147:ALA:HB3	2.21	0.55
1:E:224:LEU:HG	1:E:237:ASN:ND2	2.22	0.55
1:A:226:GLY:HA3	1:A:235:GLY:N	2.22	0.54
1:C:256:ASP:O	1:C:259:ALA:HB3	2.06	0.54
1:A:294:ARG:NH2	1:D:291:ASN:H	2.05	0.54
1:A:292:GLU:C	1:C:294:ARG:HB3	2.28	0.54
1:B:133:THR:O	1:B:137:LEU:HG	2.06	0.54
1:A:361:LEU:HG	1:A:362:CYS:N	2.23	0.54
1:B:152:ARG:CG	1:B:179:GLN:HG3	2.37	0.54
1:B:336:PHE:HE1	1:B:369:ALA:HB3	1.72	0.54
1:D:280:ARG:NH2	1:E:262:ILE:HD12	1.95	0.54
1:D:336:PHE:HE1	1:D:369:ALA:HB3	1.72	0.54
1:B:258:ILE:HG21	1:B:275:ILE:HD13	1.88	0.54
1:G:258:ILE:HG21	1:G:275:ILE:HD13	1.89	0.54
1:A:331:MET:HG3	1:A:372:ARG:HH22	1.71	0.54
1:C:130:ARG:HG3	1:D:271:SER:CB	2.37	0.54
1:E:317:LYS:HZ1	1:F:266:THR:HA	1.73	0.54
1:B:307:ILE:HG22	1:B:310:GLY:O	2.08	0.54
1:C:223:LEU:O	1:C:236:LEU:HG	2.08	0.54
1:D:229:THR:HG23	1:D:230:GLY:H	1.71	0.54
1:D:206:TYR:HE1	1:E:141:GLY:C	2.11	0.54
1:F:122:PRO:HB3	1:F:124:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ARG:CA	1:F:263:TYR:CE1	2.91	0.54
1:A:192:ALA:H	1:A:358:LEU:HB3	1.71	0.54
1:C:131:ARG:HD3	1:C:132:LEU:H	1.71	0.54
1:D:275:ILE:O	1:D:313:VAL:HG13	2.08	0.54
1:C:210:ARG:NH1	1:D:372:ARG:NH2	2.55	0.54
1:A:200:ALA:HA	1:A:202:MET:HE1	1.88	0.54
1:A:292:GLU:HG2	1:A:294:ARG:CZ	2.38	0.54
1:A:336:PHE:CE1	1:A:369:ALA:HB3	2.36	0.54
1:C:177:SER:HB2	1:C:179:GLN:HE21	1.73	0.54
1:C:254:ARG:HB3	1:C:381:PHE:CE2	2.42	0.54
1:D:329:PHE:O	1:D:331:MET:N	2.40	0.54
1:C:301:GLN:CB	1:D:309:TRP:HA	2.37	0.54
1:E:186:ILE:HD12	1:E:366:LEU:HD12	1.90	0.54
1:A:262:ILE:HD12	1:A:309:TRP:CD1	2.43	0.53
1:A:291:ASN:HB2	1:D:292:GLU:OE2	2.08	0.53
1:D:191:GLN:HA	1:D:358:LEU:O	2.07	0.53
1:E:279:PRO:HG2	1:E:317:LYS:HD3	1.90	0.53
1:E:317:LYS:HZ2	1:F:269:GLU:C	2.11	0.53
1:C:279:PRO:HD2	1:C:317:LYS:HB3	1.89	0.53
1:G:203:LEU:HG	1:G:206:TYR:CD2	2.38	0.53
1:A:154:GLU:HG3	1:A:155:VAL:HG23	1.91	0.53
1:B:258:ILE:O	1:B:262:ILE:HG13	2.07	0.53
1:C:244:ASP:HB2	1:C:264:GLN:NE2	2.23	0.53
1:D:229:THR:CG2	1:D:232:ASN:ND2	2.71	0.53
1:B:263:TYR:O	1:B:266:THR:N	2.40	0.53
1:B:300:PRO:HA	1:C:309:TRP:CE3	2.43	0.53
1:E:193:SER:HB3	1:F:178:LYS:HZ3	1.72	0.53
1:E:286:ALA:O	1:E:298:GLY:HA2	2.08	0.53
1:E:130:ARG:HH12	1:E:304:THR:HB	1.73	0.53
1:A:203:LEU:HD12	1:B:148:LEU:HD22	1.90	0.53
1:B:301:GLN:HA	1:C:309:TRP:HA	1.90	0.53
1:F:133:THR:HG22	1:F:136:ASP:CB	2.38	0.53
1:A:125:ILE:HG22	1:A:212:MET:HG3	1.86	0.53
1:E:317:LYS:HB3	1:F:269:GLU:OE2	2.09	0.53
1:A:129:LEU:CG	1:A:130:ARG:H	2.20	0.53
1:A:202:MET:CE	1:B:144:SER:H	2.22	0.53
1:F:275:ILE:CB	1:F:313:VAL:HG12	2.36	0.53
1:A:280:ARG:HH21	1:B:311:LEU:HD12	1.73	0.53
1:B:306:ASN:O	1:B:308:MET:N	2.42	0.53
1:D:224:LEU:HG	1:D:237:ASN:ND2	2.24	0.53
1:E:336:PHE:HD1	1:E:367:ALA:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:ASP:O	1:F:259:ALA:HB3	2.08	0.53
1:F:152:ARG:HB2	1:F:371:TYR:O	2.08	0.53
1:G:252:ASP:HB2	1:G:256:ASP:CG	2.29	0.52
1:A:203:LEU:HD13	1:B:148:LEU:HD22	1.91	0.52
1:A:313:VAL:HG12	1:A:314:VAL:N	2.24	0.52
1:B:131:ARG:HA	1:B:131:ARG:NH1	2.23	0.52
1:D:224:LEU:HD12	1:D:236:LEU:HB2	1.90	0.52
1:D:306:ASN:CB	1:D:313:VAL:HB	2.25	0.52
1:A:342:THR:HG22	1:A:343:VAL:N	2.24	0.52
1:C:280:ARG:NE	1:D:263:TYR:HE2	2.06	0.52
1:G:122:PRO:HG2	1:G:123:GLY:H	1.75	0.52
1:A:152:ARG:HB2	1:A:371:TYR:O	2.10	0.52
1:D:193:SER:HB3	1:E:178:LYS:HD3	1.91	0.52
1:C:263:TYR:O	1:C:266:THR:N	2.40	0.52
1:F:361:LEU:HG	1:F:362:CYS:H	1.74	0.52
1:A:128:GLY:HA2	1:A:130:ARG:NH1	2.24	0.52
1:C:317:LYS:NZ	1:D:270:PHE:O	2.42	0.52
1:C:336:PHE:HE1	1:C:369:ALA:HB3	1.73	0.52
1:G:349:ASP:OD2	1:G:350:ARG:HG2	2.10	0.52
1:C:275:ILE:HB	1:C:313:VAL:HG13	1.92	0.52
1:E:317:LYS:HG3	1:F:269:GLU:C	2.30	0.52
1:G:189:TRP:HZ3	1:G:191:GLN:HE21	1.57	0.52
1:A:336:PHE:HD1	1:A:367:ALA:O	1.93	0.52
1:B:283:HIS:O	1:B:286:ALA:HB3	2.10	0.52
1:D:270:PHE:CZ	1:D:372:ARG:CZ	2.93	0.52
1:D:239:VAL:HG21	1:D:370:HIS:CG	2.45	0.52
1:G:270:PHE:HE1	1:G:372:ARG:CZ	2.22	0.52
1:A:203:LEU:HD21	1:A:207:ILE:HD11	1.92	0.52
1:C:275:ILE:HG23	1:C:326:VAL:HG22	1.92	0.52
1:A:280:ARG:HG2	1:B:310:GLY:N	2.24	0.51
1:B:254:ARG:HB3	1:B:381:PHE:CE2	2.44	0.51
1:B:254:ARG:HB3	1:B:381:PHE:HE2	1.75	0.51
1:C:306:ASN:HD22	1:C:313:VAL:C	2.13	0.51
1:G:148:LEU:HD13	1:G:336:PHE:CD2	2.45	0.51
1:G:194:ARG:HD2	1:G:347:ARG:NH2	2.26	0.51
1:B:336:PHE:HB2	1:B:367:ALA:HB3	1.92	0.51
1:D:297:PHE:CE2	1:D:308:MET:HG3	2.44	0.51
1:E:133:THR:O	1:E:135:ARG:N	2.42	0.51
1:E:275:ILE:CD1	1:E:308:MET:HB3	2.38	0.51
1:A:260:HIS:O	1:A:263:TYR:HB3	2.10	0.51
1:A:347:ARG:HG2	1:A:358:LEU:CG	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ASN:HB2	1:C:313:VAL:CB	2.26	0.51
1:D:334:GLN:HE21	1:D:371:TYR:HE1	1.59	0.51
1:C:279:PRO:HG3	1:C:315:PRO:O	2.10	0.51
1:E:308:MET:C	1:E:310:GLY:N	2.63	0.51
1:G:299:GLY:O	1:G:303:PHE:HB2	2.11	0.51
1:C:268:SER:O	1:C:269:GLU:HB2	2.09	0.51
1:E:139:ALA:O	1:E:334:GLN:HG3	2.11	0.51
1:A:196:VAL:O	1:A:200:ALA:HB3	2.10	0.51
1:A:200:ALA:HA	1:A:202:MET:CE	2.40	0.51
1:A:263:TYR:HE1	1:F:279:PRO:HB2	1.75	0.51
1:A:269:GLU:OE2	1:F:317:LYS:HB2	2.11	0.51
1:D:119:MET:HG3	1:D:120:GLN:H	1.76	0.51
1:D:307:ILE:HG22	1:D:310:GLY:HA2	1.92	0.51
1:G:258:ILE:HG21	1:G:308:MET:HE1	1.92	0.51
1:A:206:TYR:CE1	1:B:141:GLY:HA2	2.46	0.51
1:E:124:ILE:O	1:E:124:ILE:HG22	2.11	0.51
1:E:301:GLN:HG3	1:F:309:TRP:HA	1.93	0.51
1:E:352:ASN:HA	1:E:357:MET:HB3	1.93	0.51
1:F:126:MET:HG3	1:F:129:LEU:HD21	1.92	0.51
1:A:358:LEU:HD23	1:A:360:ILE:HG13	1.92	0.51
1:C:121:ILE:HB	1:C:122:PRO:CD	2.35	0.51
1:F:235:GLY:O	1:F:236:LEU:C	2.48	0.51
1:G:125:ILE:HD12	1:G:125:ILE:N	2.23	0.51
1:C:306:ASN:CB	1:C:313:VAL:HB	2.25	0.51
1:E:314:VAL:HG12	1:E:316:THR:OG1	2.11	0.51
1:B:258:ILE:HD11	1:B:381:PHE:CZ	2.46	0.50
1:C:244:ASP:CG	1:C:246:SER:HB3	2.32	0.50
1:A:263:TYR:CZ	1:F:280:ARG:HA	2.46	0.50
1:F:353:PHE:CD2	1:G:359:THR:HG22	2.46	0.50
1:G:183:VAL:HG22	1:G:367:ALA:HB2	1.93	0.50
1:C:258:ILE:N	1:C:258:ILE:HD12	2.25	0.50
1:E:134:ILE:CD1	1:E:316:THR:HG21	2.41	0.50
1:G:139:ALA:HB3	1:G:334:GLN:CB	2.41	0.50
1:B:208:ASN:O	1:B:212:MET:HG2	2.12	0.50
1:F:258:ILE:HG21	1:F:308:MET:HE1	1.94	0.50
1:F:275:ILE:HD12	1:F:313:VAL:CG1	2.41	0.50
1:F:316:THR:C	1:F:318:ALA:H	2.14	0.50
1:B:193:SER:O	1:B:358:LEU:HD22	2.12	0.50
1:B:280:ARG:HB2	1:C:263:TYR:CE1	2.47	0.50
1:D:259:ALA:CB	1:D:309:TRP:HE1	2.25	0.50
1:F:305:SER:HB2	1:F:315:PRO:CD	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:PRO:HD3	1:G:316:THR:O	2.12	0.50
1:E:301:GLN:NE2	1:F:309:TRP:HD1	2.08	0.50
1:A:129:LEU:O	1:A:130:ARG:CD	2.49	0.50
1:A:282:TRP:HA	1:A:285:ILE:HD12	1.93	0.50
1:A:313:VAL:HG12	1:A:314:VAL:H	1.76	0.50
1:C:277:LEU:HD11	1:C:308:MET:HE1	1.93	0.50
1:G:202:MET:CG	1:G:203:LEU:H	2.23	0.50
1:G:336:PHE:CE1	1:G:369:ALA:HB3	2.46	0.50
1:D:135:ARG:HH12	1:D:335:VAL:HG11	1.76	0.50
1:F:354:VAL:HG12	1:G:189:TRP:CG	2.47	0.50
1:G:268:SER:O	1:G:269:GLU:HB2	2.12	0.50
1:F:305:SER:HB3	1:F:313:VAL:HG23	1.94	0.50
1:G:148:LEU:CD1	1:G:336:PHE:CG	2.95	0.50
1:G:282:TRP:CE2	1:G:313:VAL:HG11	2.47	0.50
1:A:262:ILE:HD12	1:A:309:TRP:HD1	1.76	0.49
1:C:194:ARG:HG3	1:C:347:ARG:HH12	1.77	0.49
1:F:132:LEU:O	1:F:133:THR:HG23	2.11	0.49
1:A:336:PHE:HB2	1:A:367:ALA:HB3	1.93	0.49
1:D:260:HIS:O	1:D:263:TYR:HB3	2.12	0.49
1:D:219:GLU:HG3	1:D:366:LEU:CD1	2.42	0.49
1:G:203:LEU:CA	1:G:206:TYR:HB3	2.40	0.49
1:B:297:PHE:CG	1:B:298:GLY:N	2.80	0.49
1:D:280:ARG:NH1	1:E:309:TRP:CB	2.75	0.49
1:E:279:PRO:HG2	1:E:317:LYS:CD	2.43	0.49
1:A:336:PHE:HZ	1:A:371:TYR:OH	1.95	0.49
1:D:150:TYR:HE1	1:D:152:ARG:HD3	1.77	0.49
1:E:296:ILE:HG22	1:E:297:PHE:HD1	1.77	0.49
1:G:206:TYR:C	1:G:206:TYR:CD1	2.84	0.49
1:A:196:VAL:O	1:A:203:LEU:HD22	2.12	0.49
1:A:301:GLN:CG	1:A:302:ALA:H	2.21	0.49
1:D:191:GLN:O	1:E:151:VAL:HG13	2.12	0.49
1:E:306:ASN:O	1:E:308:MET:N	2.46	0.49
1:G:206:TYR:CE1	1:G:210:ARG:HB2	2.47	0.49
1:G:148:LEU:HD11	1:G:336:PHE:CG	2.48	0.49
1:A:224:LEU:HD13	1:A:237:ASN:ND2	2.27	0.49
1:A:349:ASP:O	1:A:352:ASN:HB2	2.12	0.49
1:A:288:LEU:HB2	1:A:297:PHE:HE1	1.78	0.49
1:B:253:THR:OG1	1:B:255:ALA:HB3	2.13	0.49
1:B:254:ARG:HB2	1:B:285:ILE:HG12	1.93	0.49
1:B:308:MET:HG2	1:B:309:TRP:CD1	2.48	0.49
1:B:279:PRO:HG2	1:B:317:LYS:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:ILE:HD12	1:D:366:LEU:HD12	1.95	0.49
1:F:127:PRO:O	1:F:129:LEU:HD22	2.12	0.49
1:F:305:SER:HB3	1:F:313:VAL:O	2.13	0.49
1:A:219:GLU:HG3	1:A:366:LEU:CD1	2.41	0.49
1:D:133:THR:CB	1:D:314:VAL:HG13	2.43	0.49
1:F:150:TYR:HE1	1:F:152:ARG:HB3	1.77	0.49
1:D:292:GLU:HA	1:F:294:ARG:HH11	1.78	0.49
1:G:336:PHE:HE1	1:G:369:ALA:N	2.11	0.49
1:B:317:LYS:HZ1	1:C:266:THR:HA	1.74	0.48
1:E:129:LEU:HB2	1:F:330:ASP:OD2	2.12	0.48
1:E:130:ARG:HG3	1:E:131:ARG:CG	2.43	0.48
1:F:205:SER:HA	1:F:208:ASN:ND2	2.27	0.48
1:A:336:PHE:CE1	1:A:369:ALA:HB2	2.48	0.48
1:B:239:VAL:HG21	1:B:370:HIS:CG	2.48	0.48
1:C:336:PHE:HE1	1:C:369:ALA:CB	2.27	0.48
1:D:263:TYR:O	1:D:266:THR:N	2.39	0.48
1:E:188:HIS:HD2	1:E:362:CYS:HB3	1.78	0.48
1:G:191:GLN:HA	1:G:358:LEU:O	2.13	0.48
1:G:202:MET:HG2	1:G:203:LEU:H	1.78	0.48
1:A:289:LYS:CA	1:A:295:TYR:HA	2.37	0.48
1:A:297:PHE:HD1	1:A:297:PHE:O	1.97	0.48
1:A:131:ARG:CB	1:A:304:THR:HG21	2.37	0.48
1:A:352:ASN:HB3	1:A:357:MET:HB2	1.96	0.48
1:E:308:MET:SD	1:E:309:TRP:CD1	3.07	0.48
1:D:200:ALA:N	1:D:201:PRO:HD3	2.29	0.48
1:E:317:LYS:HZ3	1:F:266:THR:CA	2.20	0.48
1:G:133:THR:HG22	1:G:134:ILE:N	2.29	0.48
1:G:357:MET:O	1:G:358:LEU:HD12	2.13	0.48
1:A:283:HIS:C	1:A:285:ILE:H	2.17	0.48
1:A:258:ILE:CG2	1:A:275:ILE:HD13	2.42	0.48
1:E:134:ILE:HD12	1:E:220:GLU:HG3	1.96	0.48
1:E:308:MET:CG	1:E:309:TRP:HD1	2.26	0.48
1:C:193:SER:HB3	1:D:178:LYS:NZ	2.29	0.48
1:E:336:PHE:CE1	1:E:369:ALA:CB	2.79	0.48
1:F:288:LEU:O	1:F:296:ILE:HG12	2.14	0.48
1:F:307:ILE:HG22	1:F:307:ILE:O	2.14	0.48
1:E:202:MET:HG3	1:F:142:ARG:O	2.13	0.47
1:G:334:GLN:HG2	1:G:371:TYR:OH	2.14	0.47
1:A:304:THR:HB	1:A:315:PRO:HD2	1.96	0.47
1:C:200:ALA:HB1	1:C:204:GLN:HB2	1.94	0.47
1:D:125:ILE:HG12	1:D:212:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:ILE:HD12	1:F:366:LEU:HD12	1.96	0.47
1:D:196:VAL:HG22	1:D:203:LEU:HD21	1.96	0.47
1:E:152:ARG:HA	1:E:371:TYR:O	2.14	0.47
1:F:177:SER:HB2	1:F:179:GLN:HE21	1.80	0.47
1:B:133:THR:O	1:B:137:LEU:N	2.47	0.47
1:C:253:THR:HB	1:C:288:LEU:HD11	1.96	0.47
1:F:224:LEU:HD22	1:F:237:ASN:ND2	2.28	0.47
1:F:317:LYS:C	1:F:319:GLN:N	2.65	0.47
1:F:352:ASN:ND2	1:F:359:THR:H	2.12	0.47
1:G:216:ALA:O	1:G:220:GLU:HB2	2.14	0.47
1:G:132:LEU:CD2	1:G:135:ARG:HB3	2.45	0.47
1:E:190:VAL:O	1:E:360:ILE:HB	2.14	0.47
1:G:196:VAL:CG1	1:G:203:LEU:HD22	2.45	0.47
1:G:270:PHE:HE1	1:G:372:ARG:NE	2.13	0.47
1:A:308:MET:C	1:A:310:GLY:H	2.18	0.47
1:B:122:PRO:HD2	1:B:208:ASN:ND2	2.29	0.47
1:C:357:MET:O	1:C:358:LEU:HD12	2.15	0.47
1:D:139:ALA:O	1:D:334:GLN:HG3	2.14	0.47
1:D:211:LEU:HB3	1:D:362:CYS:HB2	1.97	0.47
1:F:347:ARG:HD2	1:F:358:LEU:HD12	1.95	0.47
1:F:336:PHE:HB2	1:F:367:ALA:HB3	1.96	0.47
1:D:218:LYS:O	1:D:222:GLN:HG2	2.14	0.47
1:E:127:PRO:CB	1:E:132:LEU:HD21	2.45	0.47
1:E:343:VAL:HG22	1:E:362:CYS:SG	2.55	0.47
1:E:346:SER:O	1:E:358:LEU:HG	2.15	0.47
1:G:153:GLU:HB3	1:G:372:ARG:HD2	1.96	0.47
1:B:235:GLY:O	1:B:236:LEU:C	2.54	0.47
1:C:133:THR:O	1:C:137:LEU:HG	2.15	0.47
1:C:279:PRO:CD	1:C:317:LYS:CA	2.92	0.47
1:F:207:ILE:HG21	1:F:360:ILE:HD13	1.97	0.47
1:G:336:PHE:HE1	1:G:369:ALA:HB3	1.80	0.47
1:A:206:TYR:CE2	1:B:334:GLN:OE1	2.68	0.47
1:F:295:TYR:HB3	1:F:299:GLY:HA2	1.97	0.47
1:F:215:LEU:HD12	1:F:362:CYS:SG	2.55	0.47
1:E:134:ILE:HD11	1:E:224:LEU:HD22	1.97	0.47
1:A:196:VAL:HG12	1:A:203:LEU:CD2	2.42	0.46
1:C:210:ARG:HH21	1:D:371:TYR:HB3	1.80	0.46
1:E:299:GLY:N	1:E:300:PRO:HD3	2.30	0.46
1:F:143:THR:OG1	1:F:144:SER:N	2.49	0.46
1:E:208:ASN:O	1:E:212:MET:HG2	2.14	0.46
1:A:177:SER:HB3	1:A:179:GLN:NE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLY:O	1:A:300:PRO:HD3	2.16	0.46
1:B:345:VAL:HG22	1:B:360:ILE:CG2	2.44	0.46
1:B:258:ILE:HD12	1:B:258:ILE:N	2.31	0.46
1:D:268:SER:O	1:D:269:GLU:HB2	2.15	0.46
1:F:313:VAL:O	1:F:313:VAL:HG23	2.15	0.46
1:D:206:TYR:CE1	1:E:141:GLY:C	2.88	0.46
1:B:150:TYR:CG	1:B:151:VAL:N	2.84	0.46
1:E:307:ILE:CG2	1:E:310:GLY:C	2.84	0.46
1:G:336:PHE:HE1	1:G:369:ALA:H	1.62	0.46
1:A:292:GLU:O	1:A:292:GLU:HG3	2.15	0.46
1:B:304:THR:HG23	1:B:305:SER:N	2.22	0.46
1:B:133:THR:HG21	1:B:314:VAL:HG13	1.97	0.46
1:D:201:PRO:HD2	1:D:202:MET:CE	2.45	0.46
1:E:286:ALA:HB1	1:E:299:GLY:N	2.28	0.46
1:C:152:ARG:HB2	1:C:371:TYR:O	2.15	0.46
1:D:294:ARG:NH1	1:F:295:TYR:HB2	2.31	0.46
1:E:200:ALA:HA	1:E:201:PRO:HD3	1.75	0.46
1:E:235:GLY:O	1:E:236:LEU:C	2.54	0.46
1:F:329:PHE:O	1:F:331:MET:N	2.49	0.46
1:G:129:LEU:O	1:G:131:ARG:N	2.49	0.46
1:D:229:THR:CG2	1:D:230:GLY:H	2.28	0.46
1:D:201:PRO:HB2	1:E:144:SER:OG	2.16	0.45
1:A:270:PHE:CE2	1:F:213:TYR:CE2	3.04	0.45
1:B:260:HIS:O	1:B:263:TYR:HB3	2.16	0.45
1:E:130:ARG:NH1	1:E:304:THR:HB	2.30	0.45
1:F:130:ARG:O	1:F:131:ARG:HB3	2.16	0.45
1:G:195:GLN:H	1:G:195:GLN:NE2	2.15	0.45
1:A:197:MET:SD	1:A:360:ILE:HD11	2.56	0.45
1:D:206:TYR:CD1	1:E:142:ARG:O	2.69	0.45
1:A:343:VAL:HG13	1:A:361:LEU:O	2.17	0.45
1:B:308:MET:C	1:B:310:GLY:H	2.19	0.45
1:C:306:ASN:O	1:C:313:VAL:N	2.43	0.45
1:E:197:MET:CE	1:E:207:ILE:HD13	2.46	0.45
1:F:336:PHE:CZ	1:F:371:TYR:OH	2.51	0.45
1:G:139:ALA:O	1:G:334:GLN:HB2	2.16	0.45
1:G:336:PHE:CZ	1:G:371:TYR:OH	2.63	0.45
1:A:201:PRO:O	1:A:204:GLN:HB3	2.16	0.45
1:C:280:ARG:NE	1:D:263:TYR:CE2	2.85	0.45
1:C:311:LEU:O	1:C:313:VAL:HG23	2.17	0.45
1:D:283:HIS:O	1:D:283:HIS:CD2	2.69	0.45
1:F:139:ALA:O	1:F:334:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:HIS:O	1:G:287:LEU:HG	2.16	0.45
1:G:316:THR:HG22	1:G:318:ALA:N	2.24	0.45
1:A:281:ASP:O	1:A:285:ILE:HG13	2.17	0.45
1:D:150:TYR:O	1:D:178:LYS:HA	2.17	0.45
1:F:142:ARG:NH1	1:F:142:ARG:HB3	2.31	0.45
1:C:235:GLY:O	1:C:236:LEU:C	2.55	0.45
1:D:297:PHE:HE2	1:D:308:MET:HG3	1.80	0.45
1:A:189:TRP:HD1	1:A:189:TRP:H	1.65	0.45
1:B:329:PHE:O	1:B:331:MET:N	2.50	0.45
1:C:279:PRO:CD	1:C:317:LYS:CB	2.92	0.45
1:E:149:GLU:HA	1:E:179:GLN:O	2.17	0.45
1:C:177:SER:HB2	1:C:179:GLN:NE2	2.31	0.45
1:E:263:TYR:O	1:E:266:THR:N	2.46	0.45
1:A:263:TYR:O	1:A:266:THR:N	2.35	0.45
1:E:192:ALA:O	1:E:357:MET:HA	2.17	0.45
1:G:286:ALA:CA	1:G:297:PHE:HZ	2.19	0.45
1:A:264:GLN:HG2	1:A:377:ILE:CD1	2.46	0.44
1:A:189:TRP:HA	1:A:361:LEU:HA	1.98	0.44
1:B:297:PHE:O	1:B:300:PRO:HD2	2.17	0.44
1:C:125:ILE:CG2	1:C:126:MET:H	2.24	0.44
1:D:357:MET:O	1:D:358:LEU:HD12	2.17	0.44
1:E:133:THR:HG22	1:E:314:VAL:HG12	1.96	0.44
1:E:224:LEU:HG	1:E:237:ASN:HD22	1.82	0.44
1:F:208:ASN:O	1:F:212:MET:HG2	2.17	0.44
1:G:177:SER:HB2	1:G:179:GLN:HE21	1.81	0.44
1:G:125:ILE:CD1	1:G:125:ILE:H	2.27	0.44
1:A:152:ARG:NE	1:A:179:GLN:HG3	2.33	0.44
1:B:317:LYS:NZ	1:C:270:PHE:O	2.47	0.44
1:D:324:PHE:HB3	1:D:381:PHE:HE1	1.82	0.44
1:E:147:ALA:C	1:E:148:LEU:HG	2.37	0.44
1:E:193:SER:HA	1:E:357:MET:HA	2.00	0.44
1:F:119:MET:HG2	1:F:121:ILE:HD13	1.98	0.44
1:C:195:GLN:HG3	1:D:149:GLU:OE1	2.17	0.44
1:C:282:TRP:CZ3	1:C:308:MET:HB2	2.53	0.44
1:E:137:LEU:HD11	1:E:314:VAL:HG21	1.98	0.44
1:F:196:VAL:HG12	1:F:207:ILE:HD11	2.00	0.44
1:G:334:GLN:HG2	1:G:371:TYR:CE1	2.52	0.44
1:B:190:VAL:HG12	1:B:191:GLN:N	2.32	0.44
1:B:279:PRO:HG3	1:B:315:PRO:O	2.17	0.44
1:B:317:LYS:HB3	1:C:269:GLU:CG	2.42	0.44
1:E:254:ARG:HB3	1:E:381:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:THR:C	1:G:268:SER:H	2.20	0.44
1:C:197:MET:HG2	1:C:358:LEU:HD21	1.98	0.44
1:C:262:ILE:HD13	1:C:311:LEU:HD12	1.99	0.44
1:C:336:PHE:HB2	1:C:367:ALA:HB3	2.00	0.44
1:D:227:ASP:HB3	1:D:229:THR:HG22	1.99	0.44
1:E:298:GLY:C	1:E:300:PRO:HD3	2.38	0.44
1:A:350:ARG:HB3	1:A:351:ASP:H	1.71	0.44
1:B:275:ILE:O	1:B:313:VAL:HA	2.18	0.44
1:B:329:PHE:C	1:B:331:MET:H	2.21	0.44
1:B:317:LYS:HE2	1:C:266:THR:HG23	2.00	0.44
1:E:150:TYR:CD1	1:E:151:VAL:N	2.86	0.44
1:G:199:ASP:O	1:G:200:ALA:HB3	2.18	0.44
1:D:129:LEU:H	1:D:130:ARG:NH2	2.15	0.44
1:E:134:ILE:HD12	1:E:220:GLU:CG	2.48	0.44
1:E:150:TYR:HD1	1:E:151:VAL:N	2.16	0.44
1:G:202:MET:CG	1:G:203:LEU:N	2.80	0.44
1:C:285:ILE:O	1:C:288:LEU:HB2	2.18	0.44
1:F:119:MET:SD	1:F:121:ILE:CG1	2.98	0.44
1:D:294:ARG:NH1	1:F:299:GLY:HA2	2.31	0.44
1:F:275:ILE:HD12	1:F:313:VAL:HG12	2.00	0.44
1:G:129:LEU:O	1:G:130:ARG:C	2.57	0.44
1:F:353:PHE:HB3	1:G:349:ASP:OD1	2.18	0.43
1:G:229:THR:CG2	1:G:230:GLY:H	2.20	0.43
1:C:275:ILE:HD12	1:C:313:VAL:CG2	2.47	0.43
1:F:258:ILE:HG21	1:F:275:ILE:HD13	2.01	0.43
1:A:263:TYR:HE1	1:F:280:ARG:N	2.13	0.43
1:F:361:LEU:CG	1:F:362:CYS:H	2.31	0.43
1:G:137:LEU:HD11	1:G:314:VAL:HG21	2.00	0.43
1:D:254:ARG:HB3	1:D:381:PHE:HE2	1.82	0.43
1:F:316:THR:C	1:F:318:ALA:N	2.71	0.43
1:A:152:ARG:CZ	1:A:179:GLN:HG3	2.47	0.43
1:B:224:LEU:CD1	1:B:237:ASN:ND2	2.81	0.43
1:C:279:PRO:CG	1:C:317:LYS:CB	2.84	0.43
1:C:279:PRO:HD3	1:C:317:LYS:CA	2.49	0.43
1:G:121:ILE:O	1:G:124:ILE:HD11	2.19	0.43
1:G:220:GLU:OE1	1:G:316:THR:HG23	2.19	0.43
1:D:253:THR:OG1	1:D:255:ALA:HB3	2.18	0.43
1:D:206:TYR:HE1	1:E:141:GLY:CA	2.31	0.43
1:A:133:THR:HB	1:A:134:ILE:H	1.37	0.43
1:B:121:ILE:HD12	1:B:122:PRO:HD2	2.00	0.43
1:D:306:ASN:OD1	1:D:315:PRO:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:SER:HA	1:E:178:LYS:NZ	2.34	0.43
1:E:317:LYS:CB	1:F:269:GLU:HG3	2.39	0.43
1:B:211:LEU:HD13	1:B:343:VAL:CG1	2.49	0.43
1:C:258:ILE:HG21	1:C:275:ILE:HD13	2.01	0.43
1:D:130:ARG:N	1:D:130:ARG:HE	2.16	0.43
1:E:256:ASP:O	1:E:259:ALA:HB3	2.19	0.43
1:E:197:MET:HB2	1:E:347:ARG:HH21	1.84	0.43
1:F:224:LEU:CD1	1:F:237:ASN:ND2	2.78	0.43
1:F:301:GLN:HB3	1:F:301:GLN:HE21	1.55	0.43
1:F:279:PRO:CD	1:F:317:LYS:HG2	2.38	0.43
1:G:275:ILE:HG12	1:G:326:VAL:HG22	2.01	0.43
1:B:143:THR:OG1	1:B:144:SER:N	2.52	0.43
1:C:254:ARG:O	1:C:258:ILE:HD13	2.19	0.43
1:C:239:VAL:HG21	1:C:370:HIS:CE1	2.53	0.43
1:A:267:GLU:C	1:F:317:LYS:HZ1	2.22	0.43
1:C:196:VAL:HG13	1:C:207:ILE:HD11	2.00	0.43
1:D:119:MET:HB2	1:D:345:VAL:H	1.84	0.43
1:E:193:SER:CB	1:F:178:LYS:HZ3	2.32	0.43
1:A:266:THR:CG2	1:F:279:PRO:CB	2.63	0.43
1:A:270:PHE:CZ	1:F:213:TYR:CE2	3.07	0.42
1:C:121:ILE:HG21	1:C:208:ASN:HD21	1.83	0.42
1:E:305:SER:C	1:E:307:ILE:N	2.71	0.42
1:E:314:VAL:C	1:E:316:THR:H	2.21	0.42
1:F:268:SER:O	1:F:269:GLU:HB2	2.18	0.42
1:E:213:TYR:HE2	1:F:270:PHE:HE2	1.66	0.42
1:F:336:PHE:HE1	1:F:369:ALA:CB	2.32	0.42
1:F:352:ASN:ND2	1:F:359:THR:N	2.62	0.42
1:A:199:ASP:O	1:A:201:PRO:HD3	2.19	0.42
1:A:334:GLN:HE21	1:A:371:TYR:HE1	1.67	0.42
1:C:304:THR:O	1:C:305:SER:HB3	2.19	0.42
1:E:311:LEU:HA	1:E:312:PRO:HD2	1.87	0.42
1:G:264:GLN:HB3	1:G:377:ILE:CD1	2.49	0.42
1:A:342:THR:O	1:A:362:CYS:HA	2.18	0.42
1:C:299:GLY:N	1:C:300:PRO:HD3	2.34	0.42
1:E:183:VAL:HG22	1:E:367:ALA:HB2	1.99	0.42
1:E:317:LYS:NZ	1:F:270:PHE:O	2.49	0.42
1:G:282:TRP:CZ2	1:G:313:VAL:HG21	2.54	0.42
1:A:245:THR:O	1:A:245:THR:HG22	2.19	0.42
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	0.42
1:B:308:MET:O	1:B:309:TRP:HB2	2.19	0.42
1:C:268:SER:O	1:C:269:GLU:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:LEU:O	1:D:236:LEU:HG	2.19	0.42
1:B:361:LEU:HG	1:B:362:CYS:N	2.35	0.42
1:C:329:PHE:O	1:C:331:MET:N	2.52	0.42
1:G:137:LEU:CD1	1:G:314:VAL:HG21	2.50	0.42
1:A:235:GLY:O	1:A:236:LEU:C	2.57	0.42
1:C:311:LEU:HA	1:C:312:PRO:HD3	1.89	0.42
1:C:336:PHE:HD1	1:C:367:ALA:O	2.03	0.42
1:E:357:MET:O	1:E:358:LEU:HD12	2.19	0.42
1:F:308:MET:HB3	1:F:313:VAL:CG1	2.49	0.42
1:C:224:LEU:HD13	1:C:237:ASN:HD21	1.84	0.42
1:B:317:LYS:HG3	1:C:269:GLU:O	2.20	0.42
1:D:141:GLY:O	1:D:336:PHE:HA	2.20	0.42
1:F:297:PHE:HZ	1:F:309:TRP:HE1	1.68	0.42
1:A:283:HIS:ND1	1:B:307:ILE:HB	2.35	0.42
1:C:275:ILE:CD1	1:C:308:MET:HE3	2.49	0.42
1:E:223:LEU:O	1:E:236:LEU:HD22	2.19	0.42
1:A:306:ASN:ND2	1:A:306:ASN:N	2.68	0.42
1:A:137:LEU:HD11	1:A:314:VAL:HG21	2.02	0.42
1:C:139:ALA:O	1:C:334:GLN:HG3	2.19	0.42
1:D:128:GLY:HA3	1:D:132:LEU:CD2	2.44	0.42
1:F:350:ARG:HA	1:G:350:ARG:HB3	2.01	0.42
1:F:336:PHE:HE1	1:F:369:ALA:HB3	1.85	0.42
1:A:206:TYR:HE2	1:A:210:ARG:CD	2.30	0.42
1:A:119:MET:HB2	1:A:345:VAL:O	2.20	0.42
1:C:275:ILE:H	1:C:313:VAL:HA	1.85	0.42
1:D:229:THR:HG23	1:D:232:ASN:ND2	2.31	0.42
1:D:235:GLY:O	1:D:236:LEU:C	2.58	0.42
1:E:192:ALA:HB3	1:E:358:LEU:HB3	2.02	0.42
1:E:239:VAL:HG21	1:E:370:HIS:CG	2.54	0.42
1:F:254:ARG:HB3	1:F:381:PHE:CE2	2.55	0.42
1:B:131:ARG:CD	1:C:271:SER:OG	2.67	0.41
1:D:249:ALA:N	1:D:252:ASP:OD2	2.46	0.41
1:D:255:ALA:HA	1:D:258:ILE:HD12	2.02	0.41
1:A:294:ARG:H	1:A:294:ARG:HG2	1.65	0.41
1:B:371:TYR:N	1:B:371:TYR:CD1	2.88	0.41
1:C:264:GLN:HB3	1:C:377:ILE:CD1	2.50	0.41
1:D:229:THR:CG2	1:D:230:GLY:N	2.78	0.41
1:E:124:ILE:O	1:E:126:MET:N	2.53	0.41
1:E:207:ILE:O	1:E:211:LEU:HD13	2.21	0.41
1:E:192:ALA:O	1:E:358:LEU:N	2.53	0.41
1:F:305:SER:OG	1:F:315:PRO:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:SER:HB3	1:A:196:VAL:CG2	2.50	0.41
1:A:200:ALA:HB1	1:A:203:LEU:HB3	2.02	0.41
1:B:336:PHE:HE1	1:B:369:ALA:CB	2.33	0.41
1:C:279:PRO:HG2	1:C:317:LYS:HG2	2.02	0.41
1:D:126:MET:HA	1:D:127:PRO:HD3	1.93	0.41
1:D:184:LYS:HG3	1:D:231:ASP:O	2.20	0.41
1:E:126:MET:HA	1:E:127:PRO:HD2	1.91	0.41
1:E:197:MET:HE2	1:E:345:VAL:HG11	2.01	0.41
1:F:121:ILE:HA	1:F:122:PRO:HD3	1.70	0.41
1:F:196:VAL:O	1:F:196:VAL:HG12	2.20	0.41
1:F:295:TYR:CB	1:F:299:GLY:HA2	2.51	0.41
1:G:131:ARG:C	1:G:133:THR:N	2.71	0.41
1:C:194:ARG:HG3	1:C:347:ARG:NH1	2.36	0.41
1:F:311:LEU:O	1:F:313:VAL:HG13	2.21	0.41
1:F:306:ASN:HA	1:F:312:PRO:HA	2.02	0.41
1:F:352:ASN:HA	1:F:357:MET:HB3	2.02	0.41
1:C:150:TYR:HE1	1:C:152:ARG:HB3	1.85	0.41
1:E:297:PHE:CG	1:E:297:PHE:O	2.73	0.41
1:F:354:VAL:HG12	1:G:189:TRP:CD2	2.55	0.41
1:G:241:THR:OG1	1:G:374:THR:HA	2.20	0.41
1:B:186:ILE:HD12	1:B:222:GLN:HG3	2.02	0.41
1:C:243:TYR:HA	1:C:264:GLN:OE1	2.20	0.41
1:C:258:ILE:H	1:C:258:ILE:CD1	2.33	0.41
1:C:345:VAL:HG13	1:C:360:ILE:HG12	2.03	0.41
1:D:222:GLN:HB3	1:D:233:LEU:HB2	2.02	0.41
1:C:317:LYS:CD	1:D:269:GLU:HA	2.38	0.41
1:F:224:LEU:HD11	1:F:319:GLN:HA	2.03	0.41
1:F:324:PHE:HD2	1:F:381:PHE:CE1	2.39	0.41
1:F:361:LEU:CG	1:F:362:CYS:N	2.82	0.41
1:B:211:LEU:HD13	1:B:343:VAL:HG11	2.02	0.41
1:C:203:LEU:O	1:C:207:ILE:HG13	2.21	0.41
1:E:137:LEU:HD21	1:E:314:VAL:HG21	2.01	0.41
1:C:258:ILE:H	1:C:258:ILE:HD12	1.86	0.41
1:D:133:THR:HB	1:D:314:VAL:CG1	2.50	0.41
1:D:301:GLN:HB3	1:D:302:ALA:H	1.64	0.41
1:F:264:GLN:HG2	1:F:377:ILE:CD1	2.51	0.41
1:G:126:MET:HA	1:G:127:PRO:HD3	1.96	0.41
1:A:124:ILE:C	1:A:125:ILE:HD13	2.39	0.41
1:A:202:MET:SD	1:B:143:THR:CA	3.07	0.41
1:C:317:LYS:C	1:C:319:GLN:N	2.72	0.41
1:C:239:VAL:HG12	1:C:373:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:PHE:CZ	1:C:379:GLY:HA3	2.55	0.41
1:D:143:THR:OG1	1:D:144:SER:N	2.54	0.41
1:D:275:ILE:HG23	1:D:326:VAL:HG22	2.03	0.41
1:F:202:MET:N	1:F:202:MET:SD	2.94	0.41
1:G:213:TYR:CD2	1:G:213:TYR:C	2.93	0.41
1:G:273:SER:H	1:G:328:GLY:HA2	1.86	0.41
1:A:119:MET:CB	1:A:345:VAL:O	2.69	0.41
1:A:202:MET:HG3	1:B:144:SER:OG	2.20	0.41
1:B:317:LYS:CE	1:C:266:THR:HG23	2.50	0.41
1:B:371:TYR:HD1	1:B:371:TYR:N	2.19	0.41
1:C:120:GLN:HG2	1:C:121:ILE:N	2.36	0.41
1:G:199:ASP:C	1:G:201:PRO:HD3	2.38	0.41
1:B:199:ASP:O	1:B:200:ALA:C	2.59	0.40
1:E:236:LEU:HD22	1:E:236:LEU:H	1.86	0.40
1:C:196:VAL:CG1	1:C:207:ILE:HD11	2.52	0.40
1:C:260:HIS:O	1:C:263:TYR:HB3	2.22	0.40
1:G:229:THR:CG2	1:G:230:GLY:N	2.72	0.40
1:G:183:VAL:HA	1:G:367:ALA:HB2	2.03	0.40
1:C:193:SER:HB3	1:D:178:LYS:HZ3	1.85	0.40
1:C:282:TRP:CZ2	1:C:306:ASN:HB3	2.56	0.40
1:D:294:ARG:NH1	1:F:300:PRO:HD3	2.37	0.40
1:A:289:LYS:HD2	1:A:293:GLY:O	2.22	0.40
1:A:303:PHE:O	1:A:304:THR:HG22	2.21	0.40
1:B:132:LEU:HD23	1:B:132:LEU:HA	1.88	0.40
1:B:258:ILE:HG21	1:B:308:MET:SD	2.61	0.40
1:C:131:ARG:HD3	1:C:132:LEU:N	2.35	0.40
1:D:210:ARG:NH1	1:D:213:TYR:HD2	2.19	0.40
1:D:258:ILE:HG21	1:D:275:ILE:HG21	2.04	0.40
1:E:120:GLN:O	1:E:122:PRO:HD3	2.22	0.40
1:E:130:ARG:C	1:E:130:ARG:HE	2.25	0.40
1:E:229:THR:HG22	1:E:232:ASN:HD22	1.86	0.40
1:F:234:GLU:O	1:F:368:LEU:HD23	2.21	0.40
1:A:258:ILE:CD1	1:A:258:ILE:N	2.76	0.40
1:A:278:ASN:HB3	1:A:281:ASP:OD2	2.22	0.40
1:B:336:PHE:HD1	1:B:367:ALA:O	2.05	0.40
1:D:229:THR:OG1	1:D:230:GLY:N	2.54	0.40
1:A:271:SER:HB3	1:F:130:ARG:HG2	2.04	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	250/282 (89%)	198 (79%)	37 (15%)	15 (6%)	2	22
1	B	250/282 (89%)	201 (80%)	32 (13%)	17 (7%)	1	20
1	C	250/282 (89%)	212 (85%)	30 (12%)	8 (3%)	5	36
1	D	250/282 (89%)	205 (82%)	33 (13%)	12 (5%)	2	28
1	E	250/282 (89%)	206 (82%)	34 (14%)	10 (4%)	3	31
1	F	250/282 (89%)	201 (80%)	39 (16%)	10 (4%)	3	31
1	G	250/282 (89%)	200 (80%)	36 (14%)	14 (6%)	2	24
All	All	1750/1974 (89%)	1423 (81%)	241 (14%)	86 (5%)	2	27

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	PRO
1	A	124	ILE
1	A	135	ARG
1	A	193	SER
1	A	350	ARG
1	B	151	VAL
1	B	201	PRO
1	B	202	MET
1	B	306	ASN
1	C	127	PRO
1	D	229	THR
1	D	284	ASN
1	D	299	GLY
1	D	301	GLN
1	E	307	ILE
1	F	304	THR
1	F	307	ILE
1	G	130	ARG

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Mol	Chain	Res	Type
1	G	200	ALA
1	G	229	THR
1	A	130	ARG
1	A	134	ILE
1	A	300	PRO
1	A	301	GLN
1	A	304	THR
1	B	127	PRO
1	B	300	PRO
1	C	269	GLU
1	D	130	ARG
1	D	230	GLY
1	D	306	ASN
1	D	330	ASP
1	E	125	ILE
1	E	230	GLY
1	F	330	ASP
1	G	133	THR
1	G	202	MET
1	G	350	ARG
1	B	132	LEU
1	B	199	ASP
1	B	230	GLY
1	B	297	PHE
1	B	301	GLN
1	B	330	ASP
1	C	121	ILE
1	C	330	ASP
1	D	269	GLU
1	E	134	ILE
1	E	236	LEU
1	E	318	ALA
1	F	269	GLU
1	F	300	PRO
1	F	305	SER
1	F	352	ASN
1	G	122	PRO
1	G	230	GLY
1	G	240	ALA
1	G	267	GLU
1	G	269	GLU
1	A	227	ASP

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Mol	Chain	Res	Type
1	A	240	ALA
1	A	284	ASN
1	B	287	LEU
1	B	304	THR
1	B	307	ILE
1	B	329	PHE
1	C	125	ILE
1	C	130	ARG
1	E	297	PHE
1	E	312	PRO
1	E	330	ASP
1	E	351	ASP
1	F	351	ASP
1	C	124	ILE
1	D	300	PRO
1	F	315	PRO
1	G	304	THR
1	B	310	GLY
1	D	127	PRO
1	F	309	TRP
1	G	305	SER
1	G	306	ASN
1	A	230	GLY
1	D	296	ILE
1	A	315	PRO
1	C	312	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	211/231 (91%)	188 (89%)	23 (11%)	7	31
1	B	211/231 (91%)	198 (94%)	13 (6%)	21	55
1	C	211/231 (91%)	191 (90%)	20 (10%)	10	36
1	D	211/231 (91%)	200 (95%)	11 (5%)	27	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	211/231 (91%)	195 (92%)	16 (8%)	15	48
1	F	211/231 (91%)	195 (92%)	16 (8%)	15	48
1	G	211/231 (91%)	192 (91%)	19 (9%)	11	39
All	All	1477/1617 (91%)	1359 (92%)	118 (8%)	14	46

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	124	ILE
1	A	129	LEU
1	A	130	ARG
1	A	131	ARG
1	A	133	THR
1	A	142	ARG
1	A	156	PHE
1	A	172	SER
1	A	189	TRP
1	A	190	VAL
1	A	202	MET
1	A	203	LEU
1	A	217	LEU
1	A	224	LEU
1	A	250	THR
1	A	287	LEU
1	A	290	ASP
1	A	297	PHE
1	A	303	PHE
1	A	306	ASN
1	A	309	TRP
1	A	358	LEU
1	B	129	LEU
1	B	130	ARG
1	B	132	LEU
1	B	136	ASP
1	B	151	VAL
1	B	172	SER
1	B	177	SER
1	B	201	PRO
1	B	202	MET
1	B	250	THR

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Mol	Chain	Res	Type
1	B	268	SER
1	B	297	PHE
1	B	307	ILE
1	C	126	MET
1	C	129	LEU
1	C	130	ARG
1	C	131	ARG
1	C	156	PHE
1	C	172	SER
1	C	188	HIS
1	C	202	MET
1	C	210	ARG
1	C	224	LEU
1	C	234	GLU
1	C	250	THR
1	C	256	ASP
1	C	280	ARG
1	C	288	LEU
1	C	301	GLN
1	C	303	PHE
1	C	306	ASN
1	C	317	LYS
1	C	346	SER
1	D	130	ARG
1	D	133	THR
1	D	172	SER
1	D	202	MET
1	D	210	ARG
1	D	215	LEU
1	D	250	THR
1	D	288	LEU
1	D	295	TYR
1	D	301	GLN
1	D	309	TRP
1	E	126	MET
1	E	131	ARG
1	E	150	TYR
1	E	151	VAL
1	E	172	SER
1	E	188	HIS
1	E	202	MET
1	E	229	THR

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Mol	Chain	Res	Type
1	E	250	THR
1	E	279	PRO
1	E	280	ARG
1	E	303	PHE
1	E	304	THR
1	E	305	SER
1	E	306	ASN
1	E	358	LEU
1	F	120	GLN
1	F	121	ILE
1	F	125	ILE
1	F	133	THR
1	F	145	SER
1	F	156	PHE
1	F	172	SER
1	F	188	HIS
1	F	193	SER
1	F	202	MET
1	F	250	THR
1	F	280	ARG
1	F	301	GLN
1	F	303	PHE
1	F	346	SER
1	F	354	VAL
1	G	120	GLN
1	G	121	ILE
1	G	130	ARG
1	G	131	ARG
1	G	136	ASP
1	G	172	SER
1	G	188	HIS
1	G	195	GLN
1	G	196	VAL
1	G	198	ASP
1	G	205	SER
1	G	206	TYR
1	G	245	THR
1	G	256	ASP
1	G	301	GLN
1	G	303	PHE
1	G	311	LEU
1	G	359	THR

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Mol	Chain	Res	Type
1	G	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	179	GLN
1	A	191	GLN
1	A	204	GLN
1	A	237	ASN
1	A	301	GLN
1	A	306	ASN
1	A	334	GLN
1	A	352	ASN
1	B	208	ASN
1	B	237	ASN
1	B	334	GLN
1	B	352	ASN
1	C	179	GLN
1	C	208	ASN
1	C	237	ASN
1	C	306	ASN
1	C	334	GLN
1	D	179	GLN
1	D	204	GLN
1	D	208	ASN
1	D	232	ASN
1	D	283	HIS
1	D	291	ASN
1	D	334	GLN
1	E	188	HIS
1	E	204	GLN
1	E	208	ASN
1	E	232	ASN
1	E	237	ASN
1	E	306	ASN
1	F	179	GLN
1	F	208	ASN
1	F	237	ASN
1	F	301	GLN
1	F	334	GLN
1	F	352	ASN

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Mol	Chain	Res	Type
1	G	179	GLN
1	G	188	HIS
1	G	195	GLN
1	G	232	ASN
1	G	237	ASN
1	G	301	GLN
1	G	319	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	254/282 (90%)	0.50	1 (0%) 92 89	47, 95, 95, 95	0
1	B	254/282 (90%)	0.69	5 (1%) 65 60	54, 114, 114, 114	0
1	C	254/282 (90%)	0.71	8 (3%) 49 44	57, 122, 122, 122	0
1	D	254/282 (90%)	0.65	3 (1%) 79 73	50, 103, 103, 103	0
1	E	254/282 (90%)	0.66	5 (1%) 65 60	54, 114, 114, 114	0
1	F	254/282 (90%)	0.63	2 (0%) 86 81	51, 104, 104, 104	0
1	G	254/282 (90%)	0.63	4 (1%) 72 66	61, 132, 132, 132	0
All	All	1778/1974 (90%)	0.64	28 (1%) 72 66	47, 114, 132, 132	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	MET	3.3
1	G	383	SER	2.9
1	G	254	ARG	2.8
1	B	171	GLU	2.8
1	F	134	ILE	2.8
1	C	347	ARG	2.7
1	C	149	GLU	2.7
1	B	378	LYS	2.6
1	G	337	ASP	2.6
1	D	178	LYS	2.4
1	C	362	CYS	2.4
1	E	374	THR	2.4
1	E	153	GLU	2.4
1	D	149	GLU	2.3
1	C	234	GLU	2.3
1	E	271	SER	2.3
1	C	119	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	309	TRP	2.3
1	B	194	ARG	2.2
1	C	341	ALA	2.2
1	G	127	PRO	2.2
1	D	151	VAL	2.1
1	E	323	THR	2.1
1	C	272	ALA	2.1
1	B	188	HIS	2.1
1	C	180	THR	2.0
1	E	191	GLN	2.0
1	F	140	GLN	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.