



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:42 am GMT

PDB ID : 1AIP
Title : EF-TU EF-TS COMPLEX FROM THERMUS THERMOPHILUS
Authors : Wang, Y.; Jiang, Y.; Meyering-Voss, M.; Sprinzl, M.; Sigler, P.B.
Deposited on : 1997-04-22
Resolution : 3.00 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

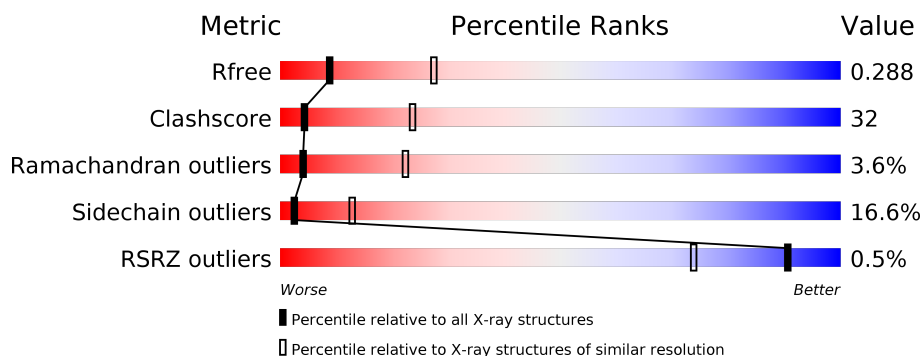
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	405	
1	B	405	
1	E	405	
1	F	405	
2	C	196	
2	D	196	

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Mol	Chain	Length	Quality of chain
2	G	196	<div><div></div><div>45%</div><div>42%</div><div>12%</div><div>..</div></div>
2	H	196	<div><div></div><div>45%</div><div>42%</div><div>11%</div><div>..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17575 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 ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2865	1810	503	541	11			
1	B	373	Total	C	N	O	S	0	0	0
			2859	1807	495	545	12			
1	E	372	Total	C	N	O	S	0	0	0
			2869	1812	502	543	12			
1	F	372	Total	C	N	O	S	0	0	0
			2841	1792	495	542	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	THR	ALA	CONFLICT	UNP P60338
B	35	THR	ALA	CONFLICT	UNP P60338
E	35	THR	ALA	CONFLICT	UNP P60338
F	35	THR	ALA	CONFLICT	UNP P60338

- Molecule 2 is a protein called ELONGATION FACTOR TS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	195	Total	C	N	O	S	0	0	0
			1544	969	276	290	9			
2	D	195	Total	C	N	O	S	0	0	0
			1513	952	268	284	9			
2	G	195	Total	C	N	O	S	0	0	0
			1546	970	279	288	9			
2	H	194	Total	C	N	O	S	0	0	0
			1523	957	274	283	9			

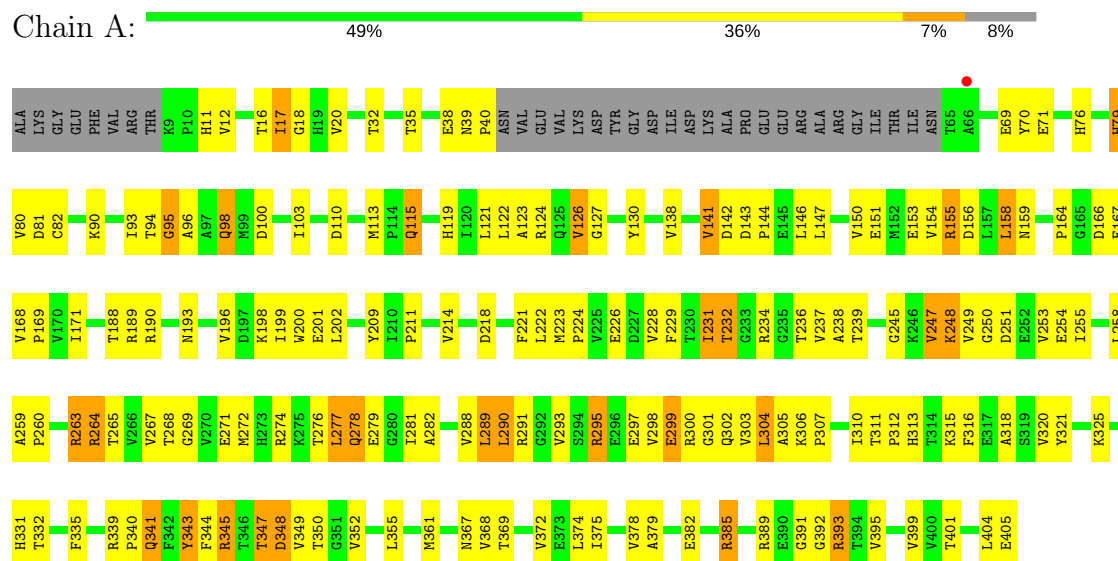
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	C	1	Total 1	O 1	0	0
3	D	4	Total 4	O 4	0	0
3	E	3	Total 3	O 3	0	0
3	G	4	Total 4	O 4	0	0
3	H	1	Total 1	O 1	0	0

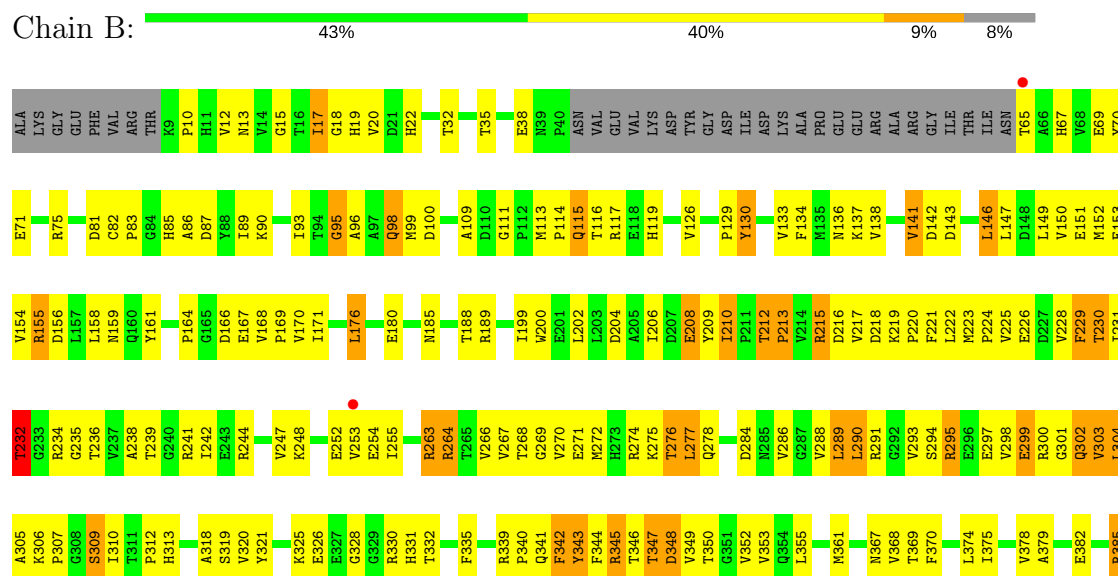
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ELONGATION FACTOR TU

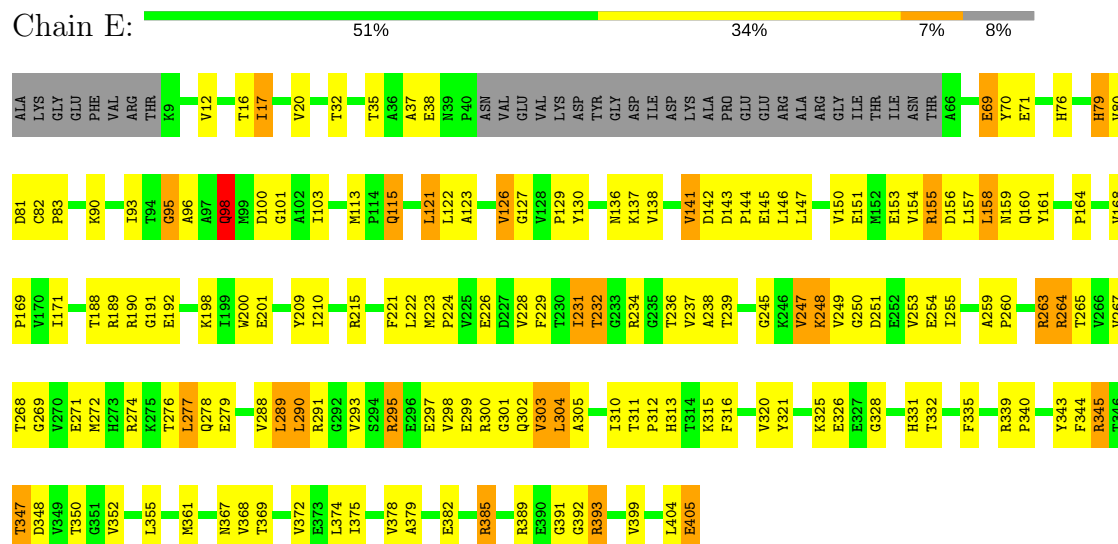


• Molecule 1: ELONGATION FACTOR TU

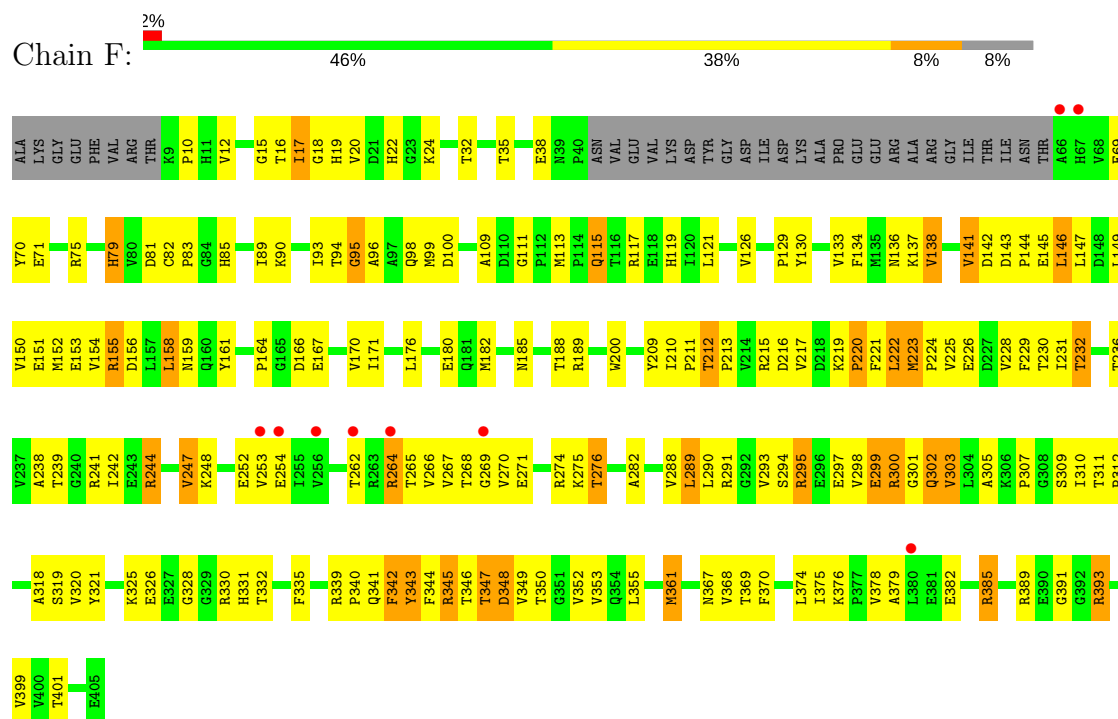




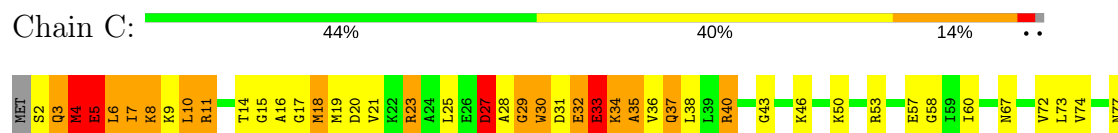
• Molecule 1: ELONGATION FACTOR TU

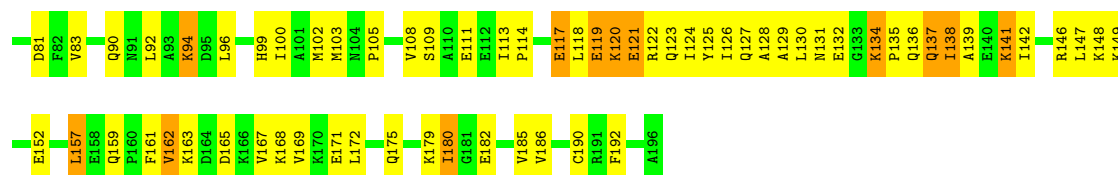


• Molecule 1: ELONGATION FACTOR TU



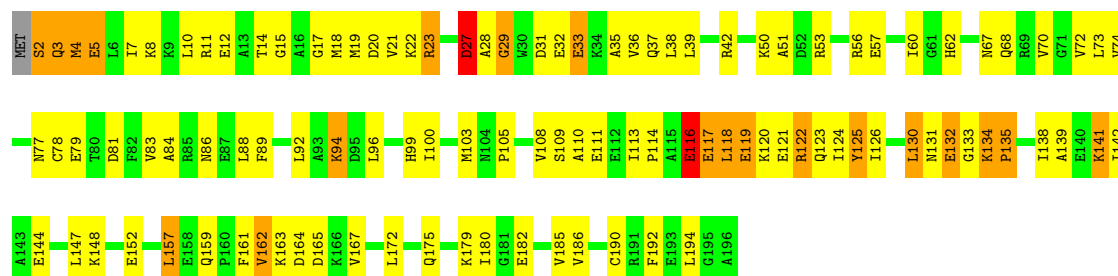
• Molecule 2: ELONGATION FACTOR TS





• Molecule 2: ELONGATION FACTOR TS

Chain D: 44% 44% 10% ..



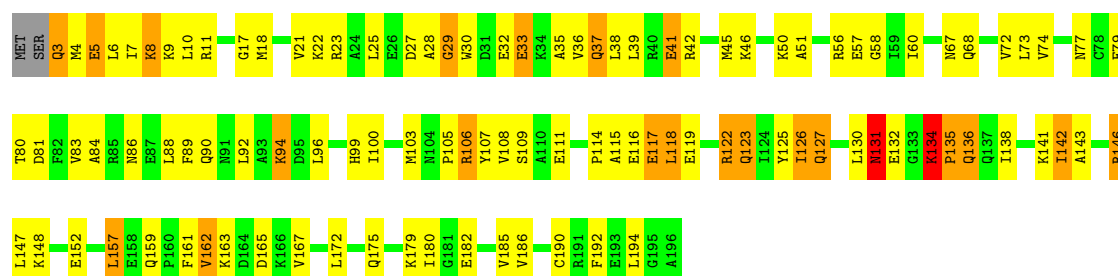
• Molecule 2: ELONGATION FACTOR TS

Chain G: 45% 42% 12% ..



• Molecule 2: ELONGATION FACTOR TS

Chain H: 45% 42% 11% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.30Å 127.50Å 123.70Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 44.39 – 2.78	Depositor EDS
% Data completeness (in resolution range)	92.0 (100.00-3.00) 90.2 (44.39-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.77Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.216 , 0.289 0.229 , 0.288	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.890	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,k,-h 0.100 for h,-k,-l 0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17575	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

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

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	0.49	1/2922 (0.0%)	0.68	0/3974
1	B	0.43	1/2915 (0.0%)	0.65	0/3965
1	E	0.49	1/2926 (0.0%)	0.69	0/3977
1	F	0.46	1/2897 (0.0%)	0.66	0/3941
2	C	0.43	0/1562	0.66	0/2094
2	D	0.41	0/1531	0.63	0/2056
2	G	0.44	0/1564	0.64	0/2096
2	H	0.43	0/1541	0.63	0/2067
All	All	0.45	4/17858 (0.0%)	0.66	0/24170

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	71	GLU	CD-OE2	7.53	1.33	1.25
1	B	71	GLU	CD-OE2	7.42	1.33	1.25
1	A	71	GLU	CD-OE2	6.74	1.33	1.25
1	E	71	GLU	CD-OE2	6.67	1.32	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2865	0	2847	168	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2859	0	2835	218	0
1	E	2869	0	2855	153	0
1	F	2841	0	2802	172	0
2	C	1544	0	1558	127	0
2	D	1513	0	1507	119	0
2	G	1546	0	1565	110	0
2	H	1523	0	1530	103	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
All	All	17575	0	17499	1122	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 32.

All (1122) 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:264:ARG:HG2	1:B:264:ARG:HH11	1.19	1.07
1:F:95:GLY:HA2	1:F:385:ARG:HH21	1.18	1.04
1:A:341:GLN:HB3	1:A:343:TYR:HE1	1.25	1.02
1:B:228:VAL:HG21	1:B:298:VAL:HG12	1.42	1.01
1:B:75:ARG:HH11	1:B:212:THR:HG23	1.26	1.00
1:B:95:GLY:HA2	1:B:385:ARG:HH21	1.24	0.99
1:A:95:GLY:HA2	1:A:385:ARG:HH21	1.27	0.98
1:B:232:THR:HG21	2:G:110:ALA:HB1	1.46	0.98
1:A:130:TYR:CE2	1:A:211:PRO:HD2	1.99	0.96
2:C:3:GLN:HA	2:C:3:GLN:HE21	1.30	0.95
1:F:341:GLN:NE2	1:F:391:GLY:H	1.64	0.95
1:F:298:VAL:HA	1:F:302:GLN:HE22	1.28	0.94
1:F:341:GLN:HE22	1:F:391:GLY:H	1.06	0.93
1:F:95:GLY:HA2	1:F:385:ARG:NH2	1.83	0.93
2:H:11:ARG:HB2	2:H:21:VAL:HG21	1.49	0.92
1:F:228:VAL:HG21	1:F:298:VAL:HG12	1.51	0.91
1:F:95:GLY:CA	1:F:385:ARG:HE	1.84	0.90
2:C:135:PRO:HG2	2:C:138:ILE:HB	1.52	0.89
1:B:224:PRO:HA	1:B:303:VAL:HG23	1.54	0.89
1:F:264:ARG:HH11	1:F:264:ARG:HG2	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:LYS:HD3	2:C:34:LYS:N	1.86	0.89
1:A:263:ARG:HH12	1:A:297:GLU:HB3	1.37	0.88
1:B:95:GLY:HA2	1:B:385:ARG:NH2	1.88	0.88
1:F:224:PRO:HA	1:F:303:VAL:HG23	1.57	0.87
2:H:161:PHE:CE2	2:H:163:LYS:HB2	2.10	0.87
2:C:33:GLU:CD	2:C:33:GLU:H	1.79	0.86
1:F:368:VAL:HG12	1:F:369:THR:H	1.38	0.86
1:A:224:PRO:HA	1:A:303:VAL:HG23	1.56	0.86
2:D:3:GLN:HG2	2:D:4:MET:H	1.41	0.85
2:C:73:LEU:HG	2:D:73:LEU:HG	1.59	0.85
1:E:255:ILE:HD12	1:E:263:ARG:HG2	1.59	0.85
1:B:306:LYS:O	1:B:309:SER:HB2	1.75	0.85
1:E:224:PRO:HA	1:E:303:VAL:HG23	1.57	0.85
2:D:130:LEU:HD13	2:D:135:PRO:HA	1.57	0.85
2:C:121:GLU:HA	2:C:124:ILE:HD12	1.57	0.84
2:D:122:ARG:HH21	2:D:126:ILE:HD11	1.41	0.84
2:D:125:TYR:HE2	2:D:147:LEU:HD23	1.41	0.84
2:C:33:GLU:O	2:C:37:GLN:HB2	1.78	0.83
2:C:6:LEU:HD22	2:C:25:LEU:HD22	1.61	0.83
1:A:341:GLN:HB3	1:A:343:TYR:CE1	2.13	0.83
2:G:146:ARG:HH11	2:G:146:ARG:HG3	1.42	0.83
2:H:3:GLN:HE22	2:H:30:TRP:HE3	1.24	0.83
1:B:368:VAL:HG12	1:B:369:THR:H	1.41	0.83
1:B:86:ALA:O	1:B:89:ILE:HG22	1.79	0.83
2:H:122:ARG:O	2:H:125:TYR:HB2	1.79	0.83
1:F:141:VAL:HG21	1:F:147:LEU:HD21	1.61	0.82
2:H:21:VAL:O	2:H:25:LEU:HD12	1.78	0.82
2:H:125:TYR:HA	2:H:146:ARG:HH12	1.44	0.82
1:B:95:GLY:N	1:B:385:ARG:HE	1.76	0.82
1:E:95:GLY:HA2	1:E:385:ARG:HH21	1.43	0.82
1:F:253:VAL:HG22	1:F:254:GLU:H	1.45	0.82
2:D:161:PHE:CE2	2:D:163:LYS:HB2	2.15	0.81
1:B:95:GLY:CA	1:B:385:ARG:HE	1.92	0.81
1:B:298:VAL:HA	1:B:302:GLN:HE22	1.44	0.81
1:F:95:GLY:N	1:F:385:ARG:HE	1.77	0.81
1:E:263:ARG:HG3	1:E:264:ARG:N	1.94	0.81
2:G:73:LEU:HB2	2:G:190:CYS:HB3	1.64	0.80
1:E:343:TYR:CZ	1:E:389:ARG:HD2	2.17	0.79
1:B:141:VAL:HG21	1:B:147:LEU:HD21	1.64	0.79
1:A:16:THR:HG23	1:A:79:HIS:HE1	1.47	0.79
2:C:118:LEU:HD12	2:C:119:GLU:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:73:LEU:HB2	2:C:190:CYS:HB3	1.65	0.79
2:D:73:LEU:HB2	2:D:190:CYS:HB3	1.63	0.79
1:B:290:LEU:HB2	1:B:293:VAL:HG21	1.64	0.78
2:C:161:PHE:CE2	2:C:163:LYS:HB2	2.17	0.78
1:B:263:ARG:HH11	1:B:263:ARG:HB3	1.49	0.78
1:F:320:VAL:HG12	1:F:321:TYR:N	1.99	0.78
2:C:137:GLN:H	2:C:137:GLN:HE21	1.29	0.78
2:G:73:LEU:HG	2:H:73:LEU:HG	1.65	0.78
1:A:226:GLU:O	1:A:300:ARG:HB2	1.83	0.77
1:B:264:ARG:NH1	1:B:264:ARG:HG2	1.94	0.77
2:C:7:ILE:HG22	2:C:21:VAL:HG12	1.66	0.77
2:H:108:VAL:O	2:H:157:LEU:HD22	1.85	0.77
1:B:295:ARG:HG3	1:B:295:ARG:HH11	1.48	0.77
2:G:161:PHE:CE2	2:G:163:LYS:HB2	2.20	0.76
2:D:118:LEU:O	2:D:118:LEU:HD12	1.85	0.76
2:H:7:ILE:HD11	2:H:22:LYS:HG3	1.65	0.76
2:H:7:ILE:O	2:H:11:ARG:HB3	1.86	0.76
2:H:130:LEU:HA	2:H:134:LYS:O	1.84	0.76
1:A:368:VAL:HG12	1:A:369:THR:H	1.49	0.76
2:C:7:ILE:HG22	2:C:21:VAL:CG1	2.16	0.76
2:D:10:LEU:HD21	2:D:36:VAL:HG12	1.66	0.76
1:E:368:VAL:HG12	1:E:369:THR:H	1.50	0.76
1:B:226:GLU:O	1:B:300:ARG:HB2	1.86	0.75
1:E:226:GLU:O	1:E:300:ARG:HB2	1.86	0.75
1:F:268:THR:OG1	1:F:291:ARG:HG3	1.86	0.75
2:G:10:LEU:CD1	2:G:25:LEU:HD21	2.17	0.75
2:C:129:ALA:O	2:C:134:LYS:HB2	1.87	0.75
1:F:75:ARG:HH11	1:F:212:THR:HG23	1.52	0.75
1:B:290:LEU:HD22	1:B:290:LEU:N	2.02	0.75
2:H:125:TYR:HB3	2:H:143:ALA:HB1	1.68	0.75
2:D:10:LEU:HD12	2:D:21:VAL:HG13	1.69	0.74
1:B:320:VAL:HG12	1:B:321:TYR:H	1.52	0.74
1:F:320:VAL:HG12	1:F:321:TYR:H	1.51	0.74
1:B:115:GLN:HG2	2:D:83:VAL:CG2	2.17	0.74
1:F:115:GLN:HG2	2:H:83:VAL:CG2	2.17	0.74
2:G:3:GLN:HA	2:G:3:GLN:HE21	1.53	0.74
2:H:125:TYR:CE2	2:H:146:ARG:HD2	2.23	0.74
1:A:16:THR:HG23	1:A:79:HIS:CE1	2.23	0.73
1:F:264:ARG:HG2	1:F:264:ARG:NH1	2.03	0.73
1:B:320:VAL:HG12	1:B:321:TYR:N	2.04	0.73
1:A:115:GLN:HE21	1:A:115:GLN:H	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:TYR:CE2	1:F:209:TYR:HB3	2.23	0.73
1:E:16:THR:HG23	1:E:79:HIS:CE1	2.24	0.73
2:H:73:LEU:HB2	2:H:190:CYS:HB3	1.69	0.73
1:A:115:GLN:NE2	1:A:115:GLN:H	1.87	0.72
1:A:130:TYR:HB3	1:A:209:TYR:CE2	2.24	0.72
1:E:115:GLN:HE21	1:E:115:GLN:H	1.36	0.72
1:F:228:VAL:HG22	1:F:238:ALA:HB2	1.71	0.72
1:A:237:VAL:HG22	1:A:289:LEU:HB3	1.70	0.72
2:D:108:VAL:O	2:D:157:LEU:HD22	1.90	0.72
1:B:115:GLN:HE21	1:B:115:GLN:H	1.37	0.72
1:B:156:ASP:HA	1:B:159:ASN:HD22	1.53	0.72
1:E:320:VAL:HG12	1:E:321:TYR:N	2.05	0.72
1:F:113:MET:HB3	1:F:115:GLN:HE22	1.54	0.72
1:A:344:PHE:O	1:A:345:ARG:HB2	1.90	0.72
1:B:385:ARG:HB2	1:B:385:ARG:HH11	1.55	0.72
1:A:164:PRO:HB2	1:A:167:GLU:HB2	1.72	0.72
1:F:156:ASP:HA	1:F:159:ASN:HD22	1.53	0.71
1:A:343:TYR:CZ	1:A:389:ARG:HD2	2.25	0.71
1:F:224:PRO:HD2	1:F:241:ARG:O	1.90	0.71
1:E:16:THR:HG23	1:E:79:HIS:HE1	1.54	0.71
1:B:115:GLN:HG2	2:D:83:VAL:HG22	1.72	0.71
1:B:341:GLN:O	1:B:388:ILE:HA	1.91	0.71
1:B:164:PRO:HB2	1:B:167:GLU:HB2	1.73	0.71
1:B:268:THR:OG1	1:B:291:ARG:HG3	1.91	0.71
1:E:115:GLN:NE2	1:E:115:GLN:H	1.89	0.71
1:F:368:VAL:HG12	1:F:369:THR:N	2.06	0.71
2:C:137:GLN:H	2:C:137:GLN:NE2	1.88	0.70
1:E:237:VAL:HG22	1:E:289:LEU:HB3	1.73	0.70
2:H:7:ILE:HG23	2:H:21:VAL:HB	1.72	0.70
1:A:231:ILE:O	1:A:231:ILE:HG22	1.91	0.70
1:F:385:ARG:HH11	1:F:385:ARG:HB2	1.56	0.70
2:G:28:ALA:O	2:G:29:GLY:O	2.08	0.70
2:G:2:SER:O	2:G:6:LEU:HB2	1.91	0.70
1:F:115:GLN:H	1:F:115:GLN:HE21	1.38	0.70
1:E:385:ARG:HG3	1:E:399:VAL:HG12	1.73	0.70
1:E:231:ILE:O	1:E:231:ILE:HG22	1.89	0.70
2:C:28:ALA:O	2:C:29:GLY:O	2.10	0.70
1:B:289:LEU:C	1:B:290:LEU:HD13	2.12	0.70
1:F:342:PHE:CD1	1:F:342:PHE:N	2.57	0.70
2:D:4:MET:O	2:D:8:LYS:HB2	1.92	0.69
2:G:123:GLN:HA	2:G:126:ILE:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:O	1:B:210:ILE:HB	1.91	0.69
2:D:96:LEU:O	2:D:100:ILE:HG13	1.92	0.69
1:A:268:THR:OG1	1:A:291:ARG:HG3	1.93	0.69
2:D:122:ARG:O	2:D:125:TYR:HB2	1.93	0.69
1:E:268:THR:OG1	1:E:291:ARG:HG3	1.92	0.69
1:B:368:VAL:HG12	1:B:369:THR:N	2.08	0.69
1:F:344:PHE:O	1:F:345:ARG:HB2	1.91	0.69
2:C:149:LYS:HD2	1:E:192:GLU:O	1.93	0.69
1:A:344:PHE:O	1:A:347:THR:HG23	1.92	0.69
1:B:344:PHE:O	1:B:345:ARG:HB2	1.91	0.69
2:C:34:LYS:HD3	2:C:34:LYS:H	1.57	0.69
2:D:32:GLU:H	2:D:32:GLU:CD	1.94	0.69
1:E:344:PHE:O	1:E:347:THR:HG23	1.93	0.69
1:B:254:GLU:OE1	1:B:307:PRO:HA	1.93	0.69
1:E:222:LEU:HD23	1:E:222:LEU:C	2.14	0.68
1:B:301:GLY:HA2	1:B:347:THR:HG22	1.75	0.68
2:C:32:GLU:O	2:C:35:ALA:N	2.26	0.68
1:A:113:MET:HB3	1:A:115:GLN:HE22	1.58	0.68
1:F:143:ASP:OD1	1:F:145:GLU:HB2	1.93	0.68
1:F:115:GLN:HG2	2:H:83:VAL:HG22	1.75	0.68
1:A:313:HIS:HB3	1:A:405:GLU:OXT	1.94	0.68
1:B:115:GLN:NE2	1:B:115:GLN:H	1.91	0.68
2:C:2:SER:HB3	2:C:5:GLU:HB2	1.76	0.68
1:F:254:GLU:OE1	1:F:307:PRO:HA	1.94	0.68
2:G:108:VAL:O	2:G:157:LEU:HD22	1.94	0.68
1:B:236:THR:OG1	1:B:293:VAL:HG23	1.94	0.67
2:C:108:VAL:O	2:C:157:LEU:HD22	1.94	0.67
2:H:138:ILE:HG22	2:H:142:ILE:HD12	1.75	0.67
2:D:3:GLN:CG	2:D:4:MET:H	2.06	0.67
1:E:146:LEU:O	1:E:150:VAL:HG23	1.94	0.67
1:A:298:VAL:HA	1:A:302:GLN:HE22	1.59	0.67
2:G:123:GLN:HA	2:G:126:ILE:CG1	2.24	0.67
1:B:216:ASP:HA	1:B:219:LYS:HD2	1.77	0.67
1:A:277:LEU:HD23	1:A:278:GLN:OE1	1.95	0.67
1:B:113:MET:HB3	1:B:115:GLN:HE22	1.59	0.67
1:B:253:VAL:HG22	1:B:254:GLU:H	1.60	0.67
2:H:96:LEU:O	2:H:100:ILE:HG13	1.95	0.67
1:E:368:VAL:HG12	1:E:369:THR:N	2.09	0.67
2:G:113:ILE:HG23	2:G:114:PRO:HD2	1.76	0.67
1:A:320:VAL:HG12	1:A:321:TYR:N	2.09	0.66
2:C:6:LEU:HD13	2:C:30:TRP:CE3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ASN:O	2:D:133:GLY:N	2.26	0.66
2:G:11:ARG:HB2	2:G:21:VAL:HG21	1.77	0.66
1:F:236:THR:HG21	1:F:294:SER:C	2.16	0.66
1:A:291:ARG:HH11	1:A:291:ARG:HB2	1.60	0.66
2:C:99:HIS:HD2	2:C:162:VAL:H	1.44	0.66
2:D:134:LYS:HD2	2:D:134:LYS:N	2.11	0.66
1:F:113:MET:HB3	1:F:115:GLN:NE2	2.09	0.66
2:D:134:LYS:HB2	2:D:138:ILE:HB	1.78	0.66
2:D:23:ARG:O	2:D:27:ASP:HB2	1.94	0.66
1:A:385:ARG:HG3	1:A:399:VAL:HG12	1.77	0.66
2:D:99:HIS:HD2	2:D:162:VAL:H	1.43	0.66
1:F:318:ALA:HA	1:F:401:THR:HG23	1.78	0.66
1:E:344:PHE:O	1:E:345:ARG:HB2	1.96	0.66
2:C:6:LEU:HD13	2:C:30:TRP:HE3	1.61	0.66
1:F:115:GLN:H	1:F:115:GLN:NE2	1.94	0.65
2:G:96:LEU:O	2:G:100:ILE:HG13	1.96	0.65
1:E:113:MET:HB3	1:E:115:GLN:HE22	1.61	0.65
1:B:236:THR:HG21	1:B:294:SER:C	2.16	0.65
1:A:263:ARG:HH22	1:A:297:GLU:HG2	1.61	0.65
2:D:3:GLN:OE1	2:D:5:GLU:HB2	1.96	0.65
1:A:368:VAL:HG12	1:A:369:THR:N	2.11	0.65
1:B:113:MET:HB3	1:B:115:GLN:NE2	2.11	0.65
1:E:247:VAL:HG13	1:E:247:VAL:O	1.95	0.65
1:E:17:ILE:HD13	1:E:17:ILE:H	1.62	0.65
2:G:10:LEU:HD13	2:G:25:LEU:HD11	1.78	0.65
1:A:95:GLY:HA2	1:A:385:ARG:NH2	2.06	0.64
2:C:34:LYS:HB2	2:C:34:LYS:HZ3	1.62	0.64
1:E:290:LEU:N	1:E:290:LEU:HD22	2.11	0.64
1:E:298:VAL:HA	1:E:302:GLN:HE22	1.60	0.64
1:F:253:VAL:HG22	1:F:254:GLU:N	2.12	0.64
1:A:90:LYS:O	1:A:94:THR:HG23	1.98	0.64
1:B:267:VAL:HG12	1:B:269:GLY:H	1.62	0.64
1:A:290:LEU:N	1:A:290:LEU:HD22	2.12	0.64
1:B:141:VAL:HG21	1:B:147:LEU:CD2	2.27	0.64
1:F:141:VAL:HG21	1:F:147:LEU:CD2	2.27	0.64
1:F:228:VAL:HG22	1:F:238:ALA:CB	2.27	0.64
1:A:224:PRO:CA	1:A:303:VAL:HG23	2.28	0.64
1:B:318:ALA:HA	1:B:401:THR:HG23	1.80	0.64
2:D:134:LYS:HG3	2:D:142:ILE:HD11	1.79	0.64
2:D:3:GLN:HG2	2:D:4:MET:N	2.12	0.64
2:C:28:ALA:HB2	2:C:38:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:LEU:HD12	2:D:130:LEU:O	1.98	0.64
1:F:210:ILE:HG13	1:F:210:ILE:O	1.98	0.64
1:F:220:PRO:O	1:F:244:ARG:HG3	1.98	0.64
1:F:236:THR:OG1	1:F:293:VAL:HG23	1.98	0.64
2:C:3:GLN:HA	2:C:3:GLN:NE2	2.10	0.63
1:F:141:VAL:CG2	1:F:147:LEU:HD21	2.29	0.63
1:A:304:LEU:H	1:A:304:LEU:CD2	2.12	0.63
2:C:129:ALA:HB3	2:C:139:ALA:HB1	1.80	0.63
1:A:222:LEU:HD23	1:A:222:LEU:C	2.19	0.63
2:C:142:ILE:HG23	1:E:191:GLY:HA2	1.81	0.63
1:F:130:TYR:HE2	1:F:209:TYR:HB3	1.64	0.63
1:F:236:THR:HG21	1:F:295:ARG:N	2.13	0.63
1:A:16:THR:CG2	1:A:79:HIS:HE1	2.12	0.63
1:E:291:ARG:HB2	1:E:291:ARG:HH11	1.62	0.62
2:H:99:HIS:HD2	2:H:162:VAL:H	1.46	0.62
1:A:289:LEU:C	1:A:290:LEU:HD13	2.20	0.62
1:B:232:THR:HG21	2:G:110:ALA:CB	2.23	0.62
2:G:146:ARG:NH1	2:G:146:ARG:HG3	2.07	0.62
1:B:100:ASP:O	1:B:129:PRO:HG2	2.00	0.62
2:C:31:ASP:OD2	2:C:34:LYS:HE3	1.99	0.62
2:D:122:ARG:NH2	2:D:126:ILE:HD11	2.12	0.62
1:B:263:ARG:NH2	1:B:297:GLU:HB3	2.14	0.62
1:E:16:THR:CG2	1:E:79:HIS:HE1	2.12	0.62
1:A:263:ARG:HG3	1:A:264:ARG:N	2.13	0.62
2:H:5:GLU:HG3	2:H:9:LYS:HE2	1.82	0.62
1:A:236:THR:HG21	1:A:295:ARG:N	2.15	0.62
1:B:141:VAL:CG2	1:B:147:LEU:HD21	2.30	0.62
1:E:304:LEU:H	1:E:304:LEU:CD2	2.12	0.62
1:F:95:GLY:CA	1:F:385:ARG:NE	2.61	0.62
1:B:221:PHE:O	1:B:305:ALA:HB1	2.00	0.62
1:B:220:PRO:O	1:B:244:ARG:HG3	2.00	0.62
2:H:114:PRO:HG2	2:H:117:GLU:HB2	1.82	0.61
2:C:119:GLU:OE1	2:C:119:GLU:HA	1.99	0.61
2:D:3:GLN:CG	2:D:4:MET:N	2.64	0.61
2:D:139:ALA:HA	2:D:142:ILE:HB	1.82	0.61
1:B:304:LEU:CD2	1:B:304:LEU:H	2.12	0.61
2:G:113:ILE:CG2	2:G:114:PRO:HD2	2.29	0.61
2:G:141:LYS:O	2:G:144:GLU:HB2	2.01	0.61
2:D:121:GLU:HA	2:D:124:ILE:HD12	1.83	0.61
1:F:171:ILE:HD12	1:F:171:ILE:N	2.16	0.61
1:A:171:ILE:N	1:A:171:ILE:HD12	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:43:GLY:HA2	2:C:46:LYS:HG3	1.82	0.61
1:E:115:GLN:HG2	2:G:83:VAL:CG2	2.30	0.61
1:A:17:ILE:H	1:A:17:ILE:HD13	1.66	0.61
1:F:291:ARG:NH1	1:F:291:ARG:HB2	2.16	0.61
1:B:223:MET:CE	1:B:304:LEU:HD21	2.31	0.61
1:B:75:ARG:HH22	1:B:210:ILE:CG2	2.14	0.61
2:D:134:LYS:HB2	2:D:138:ILE:HD12	1.82	0.61
2:H:8:LYS:HG3	2:H:9:LYS:HG2	1.83	0.61
2:H:7:ILE:CD1	2:H:22:LYS:HG3	2.30	0.60
1:B:204:ASP:O	1:B:208:GLU:HG2	2.00	0.60
2:G:125:TYR:HE2	2:G:147:LEU:HD23	1.66	0.60
1:B:171:ILE:HD12	1:B:171:ILE:N	2.16	0.60
2:C:90:GLN:HE22	2:D:68:GLN:HE22	1.47	0.60
1:A:113:MET:HB3	1:A:115:GLN:NE2	2.16	0.60
1:A:263:ARG:NH1	1:A:297:GLU:HB3	2.12	0.60
2:C:31:ASP:HB3	2:C:34:LYS:NZ	2.16	0.60
1:F:164:PRO:HB2	1:F:167:GLU:HB2	1.82	0.60
1:A:295:ARG:HH11	1:A:295:ARG:HG3	1.66	0.60
1:F:95:GLY:HA2	1:F:385:ARG:CZ	2.31	0.60
2:G:10:LEU:HD12	2:G:25:LEU:HD21	1.82	0.60
1:A:255:ILE:HD12	1:A:263:ARG:HG2	1.82	0.60
2:G:114:PRO:HG2	2:G:117:GLU:HB3	1.84	0.60
2:G:136:GLN:O	2:G:138:ILE:N	2.34	0.60
1:B:228:VAL:HG22	1:B:238:ALA:HB2	1.83	0.60
2:C:96:LEU:O	2:C:100:ILE:HG13	2.02	0.60
1:B:231:ILE:HG22	1:B:231:ILE:O	2.02	0.59
2:C:14:THR:CG2	2:C:40:ARG:HH12	2.15	0.59
2:C:3:GLN:O	2:C:6:LEU:HB2	2.01	0.59
1:F:226:GLU:O	1:F:300:ARG:HB2	2.01	0.59
1:B:342:PHE:CD1	1:B:342:PHE:N	2.68	0.59
2:C:120:LYS:HZ3	2:C:121:GLU:N	2.00	0.59
1:F:100:ASP:O	1:F:129:PRO:HG2	2.02	0.59
1:A:350:THR:HB	1:A:375:ILE:HD13	1.83	0.59
2:G:57:GLU:O	2:G:77:ASN:HA	2.02	0.59
1:B:75:ARG:HH11	1:B:212:THR:CG2	2.08	0.59
2:D:19:MET:HB3	2:D:23:ARG:NH1	2.17	0.59
1:B:295:ARG:NH1	1:B:295:ARG:HG3	2.17	0.59
2:D:141:LYS:HE3	2:D:144:GLU:CB	2.33	0.59
1:F:115:GLN:HG2	2:H:83:VAL:HG23	1.83	0.59
2:D:125:TYR:HE2	2:D:147:LEU:CD2	2.14	0.59
1:F:290:LEU:CB	1:F:293:VAL:HG21	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:ASP:HB3	2:C:34:LYS:HZ1	1.67	0.59
1:A:291:ARG:NH1	1:A:291:ARG:HB2	2.16	0.59
1:A:93:ILE:C	1:A:95:GLY:H	2.07	0.59
2:C:148:LYS:O	2:C:152:GLU:HG3	2.03	0.59
2:G:99:HIS:HD2	2:G:162:VAL:H	1.51	0.59
1:A:347:THR:OG1	1:A:348:ASP:N	2.32	0.59
1:B:290:LEU:HB2	1:B:293:VAL:CG2	2.32	0.59
1:E:290:LEU:HB2	1:E:293:VAL:HG21	1.84	0.59
1:B:146:LEU:CD2	2:D:18:MET:HG3	2.33	0.58
1:E:291:ARG:HB2	1:E:291:ARG:NH1	2.18	0.58
1:A:385:ARG:HB2	1:A:385:ARG:HH11	1.68	0.58
1:E:325:LYS:HD2	1:E:331:HIS:ND1	2.18	0.58
1:E:236:THR:HG21	1:E:295:ARG:N	2.19	0.58
1:F:109:ALA:O	2:H:18:MET:HB3	2.03	0.58
2:G:34:LYS:HE3	2:G:34:LYS:N	2.19	0.58
1:B:18:GLY:HA2	1:B:119:HIS:CD2	2.38	0.58
2:D:125:TYR:CE2	2:D:147:LEU:HD23	2.30	0.58
1:E:335:PHE:CE2	1:E:361:MET:HB2	2.39	0.58
1:F:212:THR:HG22	1:F:213:PRO:HD2	1.84	0.58
1:B:154:VAL:O	1:B:158:LEU:HD12	2.04	0.58
1:E:224:PRO:CA	1:E:303:VAL:HG23	2.30	0.58
1:E:93:ILE:C	1:E:95:GLY:H	2.07	0.58
1:F:18:GLY:HA2	1:F:119:HIS:CD2	2.38	0.58
1:A:325:LYS:HD2	1:A:331:HIS:ND1	2.18	0.58
1:B:347:THR:OG1	1:B:348:ASP:N	2.34	0.58
2:C:31:ASP:O	2:C:34:LYS:NZ	2.36	0.58
2:D:2:SER:HB2	2:D:3:GLN:NE2	2.18	0.58
1:F:343:TYR:CE1	1:F:345:ARG:O	2.57	0.58
2:H:7:ILE:HG12	2:H:25:LEU:CD1	2.34	0.58
2:G:192:PHE:HB3	2:H:60:ILE:HD12	1.86	0.58
1:E:320:VAL:HG12	1:E:321:TYR:H	1.65	0.58
1:E:289:LEU:C	1:E:290:LEU:HD13	2.24	0.57
1:B:223:MET:HE2	1:B:304:LEU:HD21	1.84	0.57
2:C:19:MET:HB3	2:C:23:ARG:NH1	2.19	0.57
1:B:293:VAL:HA	1:B:297:GLU:OE1	2.03	0.57
1:F:320:VAL:CG1	1:F:321:TYR:N	2.67	0.57
1:A:221:PHE:O	1:A:305:ALA:HB1	2.04	0.57
1:F:16:THR:HG23	1:F:79:HIS:CE1	2.39	0.57
1:F:310:ILE:HD13	1:F:379:ALA:HB1	1.86	0.57
1:A:35:THR:HG21	1:A:70:TYR:HB2	1.85	0.57
2:G:135:PRO:HG2	2:G:137:GLN:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:TYR:CZ	2:H:147:LEU:HD23	2.39	0.57
2:D:3:GLN:O	2:D:7:ILE:HG13	2.04	0.57
1:E:222:LEU:HD23	1:E:223:MET:N	2.20	0.57
1:A:293:VAL:HA	1:A:297:GLU:OE1	2.04	0.57
1:E:143:ASP:OD1	1:E:145:GLU:HB2	2.04	0.57
1:E:171:ILE:N	1:E:171:ILE:HD12	2.20	0.57
1:F:221:PHE:O	1:F:305:ALA:HB1	2.05	0.57
1:F:325:LYS:HD2	1:F:331:HIS:ND1	2.19	0.57
1:B:115:GLN:HG2	2:D:83:VAL:HG23	1.87	0.57
1:B:310:ILE:HD13	1:B:379:ALA:HB1	1.87	0.57
2:C:141:LYS:N	2:C:141:LYS:HD2	2.20	0.57
1:F:95:GLY:HA2	1:F:385:ARG:HE	1.67	0.57
2:D:138:ILE:O	2:D:142:ILE:HG13	2.04	0.57
2:D:99:HIS:HE1	2:D:159:GLN:OE1	1.87	0.57
1:E:113:MET:HB3	1:E:115:GLN:NE2	2.19	0.57
1:E:122:LEU:O	1:E:126:VAL:HG13	2.05	0.57
2:G:3:GLN:CA	2:G:3:GLN:HE21	2.15	0.57
2:H:99:HIS:HE1	2:H:159:GLN:OE1	1.88	0.57
1:B:253:VAL:HG22	1:B:254:GLU:N	2.19	0.57
1:E:385:ARG:CG	1:E:385:ARG:HH11	2.17	0.57
1:F:343:TYR:HE1	1:F:345:ARG:O	1.87	0.57
1:F:385:ARG:CB	1:F:385:ARG:HH11	2.18	0.57
2:H:123:GLN:HA	2:H:123:GLN:NE2	2.19	0.57
2:H:5:GLU:CG	2:H:9:LYS:HE2	2.35	0.57
1:A:290:LEU:HB2	1:A:293:VAL:HG21	1.86	0.56
1:E:310:ILE:HD13	1:E:379:ALA:HB1	1.87	0.56
1:B:154:VAL:HG12	1:B:158:LEU:HD11	1.87	0.56
2:C:114:PRO:HG2	2:C:117:GLU:HB2	1.87	0.56
2:G:6:LEU:O	2:G:10:LEU:HB2	2.05	0.56
1:A:335:PHE:CE2	1:A:361:MET:HB2	2.39	0.56
2:G:32:GLU:O	2:G:35:ALA:N	2.38	0.56
2:H:42:ARG:HA	2:H:45:MET:CE	2.35	0.56
1:B:385:ARG:CB	1:B:385:ARG:HH11	2.18	0.56
2:C:7:ILE:HG23	2:C:25:LEU:CD1	2.36	0.56
1:E:295:ARG:HH11	1:E:295:ARG:HG3	1.71	0.56
1:F:267:VAL:HG13	1:F:288:VAL:CG1	2.36	0.56
1:F:320:VAL:CG1	1:F:321:TYR:H	2.17	0.56
1:F:342:PHE:HD1	1:F:342:PHE:N	2.02	0.56
1:A:278:GLN:HG2	1:A:279:GLU:H	1.71	0.56
2:C:34:LYS:N	2:C:34:LYS:CD	2.65	0.56
1:F:16:THR:HG23	1:F:79:HIS:HE1	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ILE:HD11	1:F:319:SER:OG	2.05	0.56
1:A:385:ARG:CG	1:A:385:ARG:HH11	2.18	0.56
1:F:95:GLY:HA2	1:F:385:ARG:NE	2.21	0.56
2:G:134:LYS:HB3	2:G:138:ILE:HG21	1.88	0.56
1:F:223:MET:HG3	1:F:242:ILE:HA	1.87	0.56
1:A:313:HIS:HD2	1:A:405:GLU:O	1.89	0.56
2:C:138:ILE:HG22	2:C:139:ALA:N	2.19	0.56
2:C:3:GLN:NE2	2:C:30:TRP:CE3	2.74	0.56
2:D:172:LEU:O	2:D:172:LEU:HD12	2.05	0.56
1:A:171:ILE:N	1:A:171:ILE:CD1	2.69	0.56
1:E:248:LYS:HB3	1:E:279:GLU:HG3	1.88	0.56
2:G:50:LYS:O	2:G:53:ARG:HG2	2.06	0.56
2:H:33:GLU:C	2:H:35:ALA:H	2.08	0.56
1:B:234:ARG:NH1	2:G:144:GLU:HG2	2.21	0.55
2:H:106:ARG:HD2	2:H:107:TYR:CE1	2.41	0.55
2:C:137:GLN:N	2:C:137:GLN:NE2	2.53	0.55
1:B:342:PHE:HA	1:B:387:ALA:O	2.06	0.55
2:C:111:GLU:CD	2:C:111:GLU:H	2.09	0.55
1:F:90:LYS:O	1:F:94:THR:HG23	2.06	0.55
2:G:135:PRO:HG2	2:G:138:ILE:HG12	1.89	0.55
2:H:17:GLY:O	2:H:21:VAL:HG23	2.07	0.55
1:B:290:LEU:HD23	1:B:293:VAL:HG21	1.89	0.55
2:D:32:GLU:OE1	2:D:32:GLU:N	2.40	0.55
2:H:5:GLU:O	2:H:9:LYS:HG3	2.07	0.55
1:A:343:TYR:N	1:A:343:TYR:CD1	2.75	0.55
1:B:343:TYR:HD2	1:B:389:ARG:NH2	2.05	0.55
1:E:293:VAL:HA	1:E:297:GLU:OE1	2.06	0.55
1:F:267:VAL:HG12	1:F:269:GLY:H	1.71	0.55
2:H:134:LYS:N	2:H:134:LYS:HD2	2.21	0.55
1:B:263:ARG:NH1	1:B:263:ARG:CB	2.70	0.55
1:B:130:TYR:CE1	1:B:164:PRO:HG3	2.42	0.55
2:C:35:ALA:O	2:C:38:LEU:N	2.38	0.55
1:E:301:GLY:HA2	1:E:347:THR:HG22	1.89	0.55
1:F:299:GLU:H	1:F:302:GLN:NE2	2.04	0.55
2:H:7:ILE:HG23	2:H:21:VAL:CB	2.37	0.55
2:C:100:ILE:HG23	2:C:105:PRO:HD2	1.89	0.55
1:A:146:LEU:O	1:A:150:VAL:HG23	2.06	0.55
1:B:289:LEU:O	1:B:290:LEU:HD13	2.06	0.55
1:B:389:ARG:HB2	1:B:393:ARG:O	2.07	0.55
1:E:267:VAL:HG13	1:E:288:VAL:HG13	1.89	0.55
2:G:10:LEU:HD11	2:G:25:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:50:LYS:NZ	2:G:53:ARG:NH1	2.55	0.54
2:H:57:GLU:O	2:H:77:ASN:HA	2.07	0.54
1:B:299:GLU:H	1:B:302:GLN:NE2	2.04	0.54
2:C:99:HIS:HE1	2:C:159:GLN:OE1	1.90	0.54
1:F:268:THR:HB	1:F:289:LEU:HD12	1.89	0.54
1:F:293:VAL:O	1:F:293:VAL:HG23	2.06	0.54
1:B:263:ARG:NH1	1:B:263:ARG:HB3	2.20	0.54
1:E:335:PHE:HA	1:E:355:LEU:HD11	1.88	0.54
2:H:8:LYS:HE2	2:H:9:LYS:NZ	2.22	0.54
1:B:263:ARG:HH11	1:B:263:ARG:CB	2.18	0.54
2:C:11:ARG:HB2	2:C:21:VAL:HG21	1.90	0.54
1:F:385:ARG:HH11	1:F:385:ARG:CG	2.20	0.54
2:G:129:ALA:O	2:G:132:GLU:HB2	2.08	0.54
2:H:3:GLN:HG2	2:H:4:MET:N	2.22	0.54
1:F:335:PHE:CE2	1:F:361:MET:HB2	2.43	0.54
1:A:271:GLU:OE2	1:A:274:ARG:HA	2.08	0.54
1:A:341:GLN:HG3	1:A:348:ASP:OD2	2.07	0.54
1:B:171:ILE:CD1	1:B:171:ILE:N	2.70	0.54
2:G:99:HIS:HE1	2:G:159:GLN:OE1	1.91	0.54
1:B:95:GLY:HA2	1:B:385:ARG:CZ	2.37	0.54
1:F:146:LEU:O	1:F:149:LEU:HB3	2.08	0.54
2:C:128:ALA:HA	2:C:131:ASN:HB2	1.89	0.53
1:A:38:GLU:HG3	1:A:200:TRP:CZ2	2.43	0.53
1:B:224:PRO:HD2	1:B:241:ARG:O	2.09	0.53
2:G:121:GLU:O	2:G:124:ILE:HB	2.08	0.53
2:G:192:PHE:CB	2:H:60:ILE:HD12	2.38	0.53
1:A:251:ASP:O	1:A:267:VAL:HG23	2.08	0.53
2:D:57:GLU:O	2:D:77:ASN:HA	2.08	0.53
1:F:385:ARG:HG3	1:F:399:VAL:HG12	1.90	0.53
1:B:146:LEU:O	1:B:149:LEU:HB3	2.08	0.53
1:E:385:ARG:HB2	1:E:385:ARG:HH11	1.72	0.53
1:F:326:GLU:C	1:F:328:GLY:H	2.10	0.53
2:G:123:GLN:CA	2:G:126:ILE:HG12	2.38	0.53
2:G:21:VAL:O	2:G:25:LEU:HD12	2.09	0.53
1:A:320:VAL:HG12	1:A:321:TYR:H	1.71	0.53
1:B:385:ARG:CG	1:B:385:ARG:HH11	2.22	0.53
2:D:3:GLN:NE2	2:D:3:GLN:H	2.07	0.53
1:E:221:PHE:O	1:E:305:ALA:HB1	2.08	0.53
1:E:347:THR:OG1	1:E:348:ASP:N	2.37	0.53
1:F:171:ILE:N	1:F:171:ILE:CD1	2.71	0.53
2:G:34:LYS:HE3	2:G:34:LYS:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:ILE:HG23	2:H:21:VAL:CG1	2.39	0.53
1:B:95:GLY:CA	1:B:385:ARG:NE	2.68	0.53
1:B:385:ARG:HG3	1:B:399:VAL:HG12	1.90	0.53
2:D:3:GLN:OE1	2:D:5:GLU:N	2.42	0.53
1:E:320:VAL:CG1	1:E:321:TYR:N	2.72	0.53
1:B:236:THR:HG21	1:B:295:ARG:N	2.24	0.53
1:E:141:VAL:HG21	1:E:147:LEU:HD21	1.90	0.53
1:E:155:ARG:NH2	1:E:168:VAL:O	2.36	0.53
2:D:10:LEU:HD21	2:D:36:VAL:CG1	2.38	0.53
1:E:115:GLN:HG2	2:G:83:VAL:HG23	1.90	0.53
1:B:236:THR:HG1	1:B:293:VAL:HG23	1.72	0.53
1:B:335:PHE:CE2	1:B:361:MET:HB2	2.44	0.53
2:C:113:ILE:CG2	2:C:114:PRO:HD2	2.39	0.53
1:E:38:GLU:HG3	1:E:200:TRP:CZ2	2.43	0.53
1:E:313:HIS:HD2	1:E:405:GLU:O	1.92	0.53
2:G:50:LYS:HZ3	2:G:53:ARG:NH1	2.07	0.53
1:A:304:LEU:N	1:A:304:LEU:CD2	2.71	0.52
2:C:17:GLY:O	2:C:20:ASP:N	2.42	0.52
1:F:17:ILE:HG22	1:F:82:CYS:HB2	1.91	0.52
1:A:310:ILE:HD13	1:A:379:ALA:HB1	1.91	0.52
1:B:304:LEU:N	1:B:304:LEU:CD2	2.73	0.52
2:H:125:TYR:HA	2:H:146:ARG:NH1	2.18	0.52
1:B:304:LEU:HD22	1:B:304:LEU:H	1.74	0.52
2:C:57:GLU:O	2:C:77:ASN:HA	2.10	0.52
1:E:290:LEU:H	1:E:290:LEU:HD22	1.73	0.52
1:A:223:MET:HB3	1:A:304:LEU:HD21	1.90	0.52
1:B:143:ASP:HB2	2:D:22:LYS:NZ	2.24	0.52
2:D:79:GLU:HB2	2:D:182:GLU:OE1	2.08	0.52
1:F:154:VAL:HG12	1:F:158:LEU:HD11	1.91	0.52
1:F:236:THR:HG1	1:F:293:VAL:HG23	1.72	0.52
2:H:42:ARG:HA	2:H:45:MET:HE1	1.92	0.52
2:C:121:GLU:HA	2:C:124:ILE:CD1	2.34	0.52
2:C:121:GLU:O	2:C:121:GLU:HG3	2.10	0.52
2:D:111:GLU:H	2:D:111:GLU:CD	2.12	0.52
1:E:385:ARG:CG	1:E:399:VAL:HG12	2.39	0.52
1:F:154:VAL:O	1:F:158:LEU:HD12	2.10	0.52
1:F:301:GLY:HA2	1:F:346:THR:OG1	2.09	0.52
1:B:93:ILE:HD11	1:B:319:SER:OG	2.09	0.52
1:B:350:THR:HB	1:B:375:ILE:HD13	1.92	0.52
1:A:249:VAL:HG12	1:A:250:GLY:N	2.25	0.52
1:E:350:THR:HB	1:E:375:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:LEU:HD21	2:H:18:MET:HG3	1.92	0.52
2:H:3:GLN:CD	2:H:6:LEU:CB	2.78	0.52
1:A:278:GLN:CD	1:A:278:GLN:H	2.12	0.52
1:B:320:VAL:CG1	1:B:321:TYR:H	2.20	0.52
1:B:343:TYR:CE1	1:B:345:ARG:O	2.63	0.52
2:D:10:LEU:HD11	2:D:39:LEU:CD1	2.40	0.52
2:C:60:ILE:HD12	2:D:192:PHE:HB3	1.90	0.52
2:H:125:TYR:HB3	2:H:143:ALA:CB	2.37	0.52
1:A:236:THR:OG1	1:A:293:VAL:HG23	2.10	0.51
2:G:128:ALA:O	2:G:132:GLU:HG3	2.09	0.51
1:F:254:GLU:HG3	1:F:264:ARG:HB3	1.91	0.51
2:G:111:GLU:CD	2:G:111:GLU:H	2.13	0.51
2:H:37:GLN:O	2:H:41:GLU:HB2	2.11	0.51
1:B:75:ARG:HH22	1:B:210:ILE:HG22	1.75	0.51
2:C:33:GLU:N	2:C:33:GLU:CD	2.47	0.51
1:E:115:GLN:HG2	2:G:83:VAL:HG22	1.92	0.51
1:B:301:GLY:CA	1:B:347:THR:HG22	2.41	0.51
1:B:86:ALA:HA	1:B:89:ILE:HG22	1.93	0.51
1:B:228:VAL:HG22	1:B:238:ALA:CB	2.40	0.51
1:B:95:GLY:HA2	1:B:385:ARG:HE	1.74	0.51
1:E:271:GLU:OE2	1:E:274:ARG:HA	2.10	0.51
1:B:222:LEU:HD23	1:B:222:LEU:C	2.31	0.51
2:D:114:PRO:HG2	2:D:117:GLU:HB2	1.93	0.51
2:D:148:LYS:O	2:D:152:GLU:HG3	2.10	0.51
1:B:17:ILE:HG22	1:B:82:CYS:HB2	1.91	0.51
1:E:35:THR:HG21	1:E:70:TYR:HB2	1.92	0.51
1:F:231:ILE:HG22	1:F:231:ILE:O	2.10	0.51
1:F:344:PHE:O	1:F:347:THR:HG23	2.11	0.51
2:D:120:LYS:O	2:D:124:ILE:HD11	2.10	0.51
1:E:90:LYS:HE3	1:E:321:TYR:CZ	2.45	0.51
2:G:135:PRO:HB2	2:G:137:GLN:OE1	2.10	0.51
1:F:226:GLU:HB3	1:F:300:ARG:HH21	1.76	0.51
1:B:267:VAL:HG13	1:B:288:VAL:HG13	1.93	0.51
1:B:301:GLY:HA2	1:B:346:THR:OG1	2.11	0.51
2:D:118:LEU:C	2:D:118:LEU:HD12	2.31	0.51
1:E:168:VAL:HG13	1:E:169:PRO:HD2	1.93	0.51
1:A:122:LEU:O	1:A:126:VAL:HG13	2.12	0.50
1:B:266:VAL:HB	1:B:291:ARG:NH1	2.25	0.50
2:C:121:GLU:CA	2:C:124:ILE:HD12	2.34	0.50
2:D:72:VAL:HA	2:D:190:CYS:O	2.12	0.50
1:E:130:TYR:CE2	1:E:209:TYR:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:LEU:HD23	1:F:289:LEU:H	1.76	0.50
1:A:343:TYR:N	1:A:343:TYR:HD1	2.09	0.50
2:G:43:GLY:HA2	2:G:46:LYS:HG3	1.92	0.50
2:C:34:LYS:H	2:C:34:LYS:CD	2.23	0.50
2:C:4:MET:O	2:C:6:LEU:N	2.44	0.50
1:F:244:ARG:HA	1:F:282:ALA:HB2	1.94	0.50
1:F:271:GLU:HG3	1:F:275:LYS:H	1.77	0.50
1:F:224:PRO:CA	1:F:303:VAL:HG23	2.38	0.50
1:A:115:GLN:HG2	2:C:83:VAL:CG2	2.41	0.50
1:E:391:GLY:C	1:E:393:ARG:H	2.14	0.50
1:F:210:ILE:O	1:F:210:ILE:CG1	2.59	0.50
2:H:28:ALA:O	2:H:29:GLY:O	2.30	0.50
1:B:224:PRO:CA	1:B:303:VAL:HG23	2.36	0.50
2:C:113:ILE:HG23	2:C:114:PRO:HD2	1.93	0.50
1:F:75:ARG:NH1	1:F:212:THR:HG23	2.23	0.50
1:F:349:VAL:CG1	1:F:350:THR:N	2.74	0.50
2:H:111:GLU:H	2:H:111:GLU:CD	2.14	0.50
2:H:127:GLN:O	2:H:131:ASN:ND2	2.44	0.50
1:B:95:GLY:HA2	1:B:385:ARG:NE	2.27	0.50
2:C:14:THR:HG22	2:C:40:ARG:HH12	1.75	0.50
1:F:38:GLU:HG3	1:F:200:TRP:CZ2	2.46	0.50
1:A:391:GLY:C	1:A:393:ARG:H	2.15	0.50
1:B:155:ARG:NH2	1:B:168:VAL:O	2.40	0.50
1:B:320:VAL:CG1	1:B:321:TYR:N	2.72	0.50
1:B:325:LYS:HD2	1:B:331:HIS:ND1	2.27	0.50
1:B:344:PHE:O	1:B:347:THR:HG23	2.11	0.50
2:C:67:ASN:OD1	2:C:67:ASN:C	2.49	0.50
1:E:304:LEU:H	1:E:304:LEU:HD22	1.77	0.50
1:E:90:LYS:HE3	1:E:321:TYR:CE1	2.46	0.50
1:A:17:ILE:HD13	1:A:103:ILE:O	2.12	0.50
2:D:7:ILE:HG23	2:D:21:VAL:HG12	1.93	0.50
1:E:150:VAL:O	1:E:153:GLU:HB2	2.12	0.50
1:E:304:LEU:N	1:E:304:LEU:CD2	2.73	0.50
1:E:343:TYR:OH	1:E:389:ARG:HD2	2.11	0.50
1:E:95:GLY:HA2	1:E:385:ARG:NH2	2.20	0.50
2:G:36:VAL:HG23	2:G:37:GLN:N	2.26	0.50
2:G:68:GLN:HE22	2:H:90:GLN:HE22	1.59	0.50
1:B:254:GLU:O	1:B:304:LEU:HA	2.12	0.50
1:B:326:GLU:C	1:B:328:GLY:H	2.15	0.50
1:E:223:MET:O	1:E:304:LEU:CD2	2.60	0.50
1:F:247:VAL:O	1:F:247:VAL:HG13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:VAL:HG13	1:B:288:VAL:CG1	2.42	0.49
1:E:17:ILE:N	1:E:17:ILE:HD13	2.27	0.49
1:E:253:VAL:HG22	1:E:254:GLU:H	1.77	0.49
2:H:130:LEU:HD13	2:H:135:PRO:C	2.31	0.49
1:A:141:VAL:HG21	1:A:147:LEU:HD21	1.94	0.49
1:A:155:ARG:NH2	1:A:168:VAL:O	2.40	0.49
1:A:190:ARG:HD3	1:A:200:TRP:CD1	2.47	0.49
1:B:35:THR:HG21	1:B:70:TYR:HB2	1.94	0.49
2:H:72:VAL:HA	2:H:190:CYS:O	2.11	0.49
1:E:249:VAL:HG12	1:E:250:GLY:N	2.28	0.49
1:F:185:ASN:HB3	1:F:188:THR:OG1	2.13	0.49
2:G:126:ILE:HD13	2:G:143:ALA:HB2	1.95	0.49
2:D:119:GLU:C	2:D:121:GLU:N	2.65	0.49
1:E:151:GLU:O	1:E:155:ARG:HG3	2.12	0.49
1:E:223:MET:HB3	1:E:304:LEU:HD21	1.94	0.49
2:H:125:TYR:HE2	2:H:147:LEU:N	2.10	0.49
1:B:275:LYS:O	1:B:276:THR:O	2.30	0.49
1:E:17:ILE:HG22	1:E:82:CYS:HB2	1.94	0.49
2:G:3:GLN:O	2:G:30:TRP:CZ3	2.65	0.49
1:A:17:ILE:HG22	1:A:82:CYS:HB2	1.95	0.49
2:C:7:ILE:O	2:C:10:LEU:N	2.45	0.49
2:H:109:SER:HA	2:H:157:LEU:HD23	1.95	0.49
1:B:86:ALA:O	1:B:87:ASP:C	2.51	0.49
1:E:236:THR:OG1	1:E:293:VAL:HG23	2.13	0.49
1:E:267:VAL:HG13	1:E:288:VAL:CG1	2.42	0.49
1:F:221:PHE:O	1:F:222:LEU:HB2	2.13	0.49
1:F:389:ARG:HB2	1:F:393:ARG:O	2.13	0.49
2:G:10:LEU:CD1	2:G:25:LEU:HD11	2.43	0.49
2:D:28:ALA:O	2:D:29:GLY:O	2.31	0.49
1:A:223:MET:CE	1:A:304:LEU:HD21	2.43	0.49
1:B:223:MET:O	1:B:304:LEU:CD2	2.60	0.49
2:C:29:GLY:O	2:C:31:ASP:N	2.41	0.49
1:E:385:ARG:NH1	1:E:385:ARG:HG3	2.28	0.49
1:F:150:VAL:O	1:F:153:GLU:HB2	2.13	0.49
1:B:264:ARG:NH1	1:B:264:ARG:CG	2.71	0.49
1:B:266:VAL:HB	1:B:291:ARG:HH11	1.77	0.49
1:B:90:LYS:HE2	1:B:321:TYR:CE1	2.48	0.49
1:B:349:VAL:CG1	1:B:350:THR:N	2.75	0.49
1:F:146:LEU:O	1:F:150:VAL:HG23	2.12	0.49
1:F:267:VAL:HG13	1:F:288:VAL:HG13	1.94	0.49
1:B:146:LEU:HD22	2:D:19:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:O	1:B:153:GLU:HB2	2.11	0.48
1:B:75:ARG:NH1	1:B:212:THR:HG23	2.09	0.48
2:C:23:ARG:O	2:C:27:ASP:N	2.38	0.48
2:D:53:ARG:HG2	2:D:53:ARG:HH11	1.78	0.48
1:E:190:ARG:HD3	1:E:200:TRP:CD1	2.48	0.48
1:F:176:LEU:O	1:F:180:GLU:HG3	2.13	0.48
1:F:312:PRO:HA	1:F:378:VAL:O	2.12	0.48
2:H:33:GLU:C	2:H:35:ALA:N	2.66	0.48
1:A:315:LYS:HA	1:A:372:VAL:O	2.12	0.48
1:B:271:GLU:HG2	1:B:274:ARG:HA	1.94	0.48
2:C:120:LYS:HG2	2:C:124:ILE:HD11	1.94	0.48
2:C:130:LEU:HA	2:C:134:LYS:O	2.14	0.48
1:E:171:ILE:N	1:E:171:ILE:CD1	2.75	0.48
1:F:155:ARG:NH2	1:F:170:VAL:HG23	2.28	0.48
2:H:25:LEU:HD22	2:H:30:TRP:CE3	2.48	0.48
1:A:151:GLU:O	1:A:155:ARG:HG3	2.13	0.48
1:A:248:LYS:HB3	1:A:279:GLU:HG3	1.94	0.48
1:B:272:MET:HB2	1:B:277:LEU:HD12	1.95	0.48
2:C:109:SER:HA	2:C:157:LEU:HD23	1.95	0.48
2:D:92:LEU:HD11	2:D:96:LEU:HD11	1.95	0.48
1:E:141:VAL:HG21	1:E:147:LEU:CD2	2.44	0.48
1:F:253:VAL:CG2	1:F:254:GLU:H	2.21	0.48
1:A:247:VAL:HG13	1:A:247:VAL:O	2.11	0.48
1:B:109:ALA:O	2:D:19:MET:HB2	2.13	0.48
1:B:343:TYR:CD1	1:B:347:THR:O	2.67	0.48
2:C:34:LYS:O	2:C:38:LEU:HB2	2.13	0.48
2:D:74:VAL:HG13	2:D:74:VAL:O	2.14	0.48
1:F:130:TYR:HE1	1:F:164:PRO:HG2	1.79	0.48
1:F:212:THR:CG2	1:F:213:PRO:HD2	2.43	0.48
2:G:35:ALA:O	2:G:38:LEU:N	2.46	0.48
2:H:114:PRO:O	2:H:118:LEU:HD12	2.14	0.48
1:A:301:GLY:HA2	1:A:347:THR:HG22	1.96	0.48
1:A:223:MET:O	1:A:304:LEU:CD2	2.62	0.48
1:B:223:MET:HG3	1:B:242:ILE:HA	1.95	0.48
1:F:341:GLN:NE2	1:F:391:GLY:N	2.47	0.48
2:G:125:TYR:CD2	2:G:146:ARG:HB3	2.48	0.48
1:A:222:LEU:HD23	1:A:223:MET:N	2.28	0.48
1:A:335:PHE:HA	1:A:355:LEU:HD11	1.95	0.48
1:B:136:ASN:CG	1:B:137:LYS:H	2.17	0.48
2:C:172:LEU:HD12	2:C:172:LEU:O	2.14	0.48
2:G:148:LYS:O	2:G:152:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:H	1:A:304:LEU:HD23	1.79	0.48
2:D:109:SER:HA	2:D:157:LEU:HD23	1.96	0.48
1:A:150:VAL:O	1:A:153:GLU:HB2	2.14	0.48
2:H:92:LEU:O	2:H:92:LEU:HD12	2.14	0.48
1:A:253:VAL:HG22	1:A:254:GLU:H	1.79	0.48
1:B:208:GLU:HB2	1:B:209:TYR:H	1.46	0.48
2:D:4:MET:O	2:D:8:LYS:CB	2.61	0.48
2:H:172:LEU:HD12	2:H:172:LEU:O	2.13	0.48
1:B:146:LEU:HD23	2:D:18:MET:HG3	1.96	0.48
2:H:148:LYS:O	2:H:152:GLU:HG3	2.13	0.48
1:A:350:THR:HB	1:A:375:ILE:CD1	2.44	0.47
2:C:159:GLN:O	2:C:169:VAL:HG23	2.14	0.47
1:F:298:VAL:HA	1:F:302:GLN:NE2	2.12	0.47
1:F:35:THR:HG21	1:F:70:TYR:HB2	1.96	0.47
2:G:6:LEU:HD23	2:G:25:LEU:CD2	2.43	0.47
1:A:231:ILE:O	1:A:231:ILE:CG2	2.61	0.47
1:A:290:LEU:HD23	1:A:293:VAL:HG21	1.95	0.47
1:A:343:TYR:CE2	1:A:348:ASP:HB2	2.48	0.47
1:E:123:ALA:O	1:E:127:GLY:N	2.47	0.47
1:E:391:GLY:O	1:E:393:ARG:N	2.47	0.47
2:H:125:TYR:CG	2:H:146:ARG:NH1	2.82	0.47
2:C:125:TYR:CE2	2:C:146:ARG:HB3	2.49	0.47
2:D:67:ASN:OD1	2:D:67:ASN:C	2.52	0.47
1:E:231:ILE:HG22	1:E:234:ARG:HG3	1.97	0.47
1:A:223:MET:HB3	1:A:304:LEU:CD2	2.45	0.47
1:A:98:GLN:HA	1:A:98:GLN:OE1	2.15	0.47
1:B:146:LEU:O	1:B:150:VAL:HG23	2.14	0.47
1:B:313:HIS:HB3	1:B:405:GLU:OXT	2.14	0.47
1:E:101:GLY:HA3	1:E:210:ILE:HD13	1.96	0.47
1:F:290:LEU:O	1:F:293:VAL:HG22	2.13	0.47
1:A:231:ILE:HD13	1:A:231:ILE:HA	1.71	0.47
2:G:100:ILE:HG23	2:G:105:PRO:HD2	1.97	0.47
2:G:31:ASP:OD1	2:G:34:LYS:NZ	2.48	0.47
1:B:38:GLU:HG3	1:B:200:TRP:CZ2	2.48	0.47
2:C:137:GLN:N	2:C:137:GLN:HE21	2.06	0.47
1:E:143:ASP:HB3	1:E:146:LEU:HG	1.95	0.47
1:E:315:LYS:HA	1:E:372:VAL:O	2.14	0.47
1:E:231:ILE:CG2	1:E:231:ILE:O	2.59	0.47
1:E:253:VAL:HG22	1:E:254:GLU:N	2.30	0.47
1:F:89:ILE:H	1:F:89:ILE:HG12	1.55	0.47
2:G:122:ARG:HG2	2:G:126:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG12	1:B:134:PHE:N	2.30	0.47
1:B:290:LEU:HD22	1:B:290:LEU:H	1.75	0.47
2:C:72:VAL:HA	2:C:190:CYS:O	2.15	0.47
2:H:115:ALA:HA	2:H:118:LEU:CD1	2.45	0.47
1:A:290:LEU:H	1:A:290:LEU:HD22	1.77	0.47
1:A:90:LYS:HE2	1:A:321:TYR:CE1	2.50	0.47
1:B:212:THR:HG22	1:B:213:PRO:HD2	1.95	0.47
1:B:221:PHE:CG	1:B:222:LEU:N	2.83	0.47
1:B:290:LEU:N	1:B:290:LEU:CD2	2.74	0.47
1:B:293:VAL:O	1:B:293:VAL:HG23	2.15	0.47
2:C:92:LEU:O	2:C:92:LEU:HD12	2.14	0.47
2:D:33:GLU:H	2:D:33:GLU:HG2	1.53	0.47
1:E:98:GLN:HA	1:E:98:GLN:OE1	2.15	0.47
2:C:34:LYS:CB	2:C:34:LYS:HZ3	2.28	0.47
2:D:116:GLU:HG3	2:D:116:GLU:H	1.51	0.47
2:D:134:LYS:HG3	2:D:142:ILE:CD1	2.44	0.47
1:F:225:VAL:HG13	1:F:238:ALA:HB1	1.96	0.47
1:F:222:LEU:HA	1:F:305:ALA:HB2	1.97	0.47
2:G:147:LEU:HA	2:G:147:LEU:HD23	1.72	0.47
1:A:231:ILE:HG22	1:A:234:ARG:HG3	1.97	0.47
1:A:385:ARG:CB	1:A:385:ARG:HH11	2.27	0.47
2:C:126:ILE:O	2:C:130:LEU:HG	2.15	0.47
2:C:32:GLU:O	2:C:35:ALA:HB3	2.15	0.47
2:G:94:LYS:HD3	2:G:94:LYS:HA	1.60	0.47
2:H:36:VAL:HG23	2:H:37:GLN:N	2.30	0.47
1:E:320:VAL:CG1	1:E:321:TYR:H	2.27	0.46
2:G:50:LYS:NZ	2:G:53:ARG:HH12	2.11	0.46
2:G:67:ASN:C	2:G:67:ASN:OD1	2.53	0.46
1:B:368:VAL:CG1	1:B:369:THR:H	2.20	0.46
1:F:216:ASP:HA	1:F:219:LYS:HD2	1.97	0.46
2:H:3:GLN:NE2	2:H:30:TRP:CE3	2.64	0.46
1:A:254:GLU:OE1	1:A:307:PRO:HA	2.15	0.46
2:C:129:ALA:HB3	2:C:139:ALA:CB	2.45	0.46
2:G:29:GLY:O	2:G:31:ASP:N	2.46	0.46
2:G:33:GLU:O	2:G:37:GLN:HB2	2.15	0.46
1:B:19:HIS:O	1:B:22:HIS:HB2	2.14	0.46
1:E:156:ASP:HA	1:E:159:ASN:HD22	1.80	0.46
1:E:290:LEU:HD23	1:E:293:VAL:HG21	1.97	0.46
1:F:295:ARG:HH11	1:F:295:ARG:HG3	1.79	0.46
1:A:123:ALA:O	1:A:127:GLY:N	2.49	0.46
1:A:267:VAL:HG13	1:A:288:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HD12	1:B:263:ARG:NH1	2.31	0.46
1:F:15:GLY:HA3	1:F:99:MET:SD	2.56	0.46
2:G:50:LYS:O	2:G:52:ASP:N	2.49	0.46
2:H:74:VAL:O	2:H:74:VAL:HG13	2.16	0.46
1:B:270:VAL:HG12	1:B:271:GLU:N	2.30	0.46
2:C:114:PRO:HG2	2:C:117:GLU:CB	2.45	0.46
2:D:135:PRO:HD2	2:D:138:ILE:HD12	1.97	0.46
1:B:143:ASP:HB2	2:D:22:LYS:HZ1	1.81	0.46
2:D:134:LYS:HB2	2:D:138:ILE:CB	2.44	0.46
1:F:136:ASN:CG	1:F:137:LYS:H	2.19	0.46
1:F:353:VAL:HG13	1:F:370:PHE:CD1	2.51	0.46
2:G:72:VAL:HA	2:G:190:CYS:O	2.16	0.46
1:A:168:VAL:HG13	1:A:169:PRO:HD2	1.97	0.46
1:A:198:LYS:O	1:A:201:GLU:HB2	2.15	0.46
1:A:295:ARG:HG3	1:A:295:ARG:NH1	2.30	0.46
1:A:304:LEU:H	1:A:304:LEU:HD22	1.79	0.46
1:A:320:VAL:CG1	1:A:321:TYR:N	2.77	0.46
1:B:130:TYR:HE1	1:B:164:PRO:CG	2.29	0.46
1:B:291:ARG:HB2	1:B:291:ARG:NH1	2.30	0.46
1:B:335:PHE:HA	1:B:355:LEU:HD11	1.98	0.46
2:G:126:ILE:HD13	2:G:126:ILE:H	1.81	0.46
2:H:127:GLN:O	2:H:131:ASN:HB2	2.15	0.46
2:G:58:GLY:O	2:H:194:LEU:CD2	2.64	0.46
1:A:143:ASP:HA	1:A:144:PRO:HD3	1.79	0.46
1:A:258:LEU:HD12	1:A:302:GLN:HG3	1.96	0.46
1:B:229:PHE:HB2	1:B:230:THR:H	1.57	0.46
1:F:228:VAL:HG21	1:F:298:VAL:CG1	2.35	0.46
1:F:350:THR:HB	1:F:375:ILE:HD13	1.98	0.46
1:F:85:HIS:ND1	1:F:85:HIS:C	2.69	0.46
1:A:154:VAL:HG12	1:A:158:LEU:HD11	1.97	0.46
1:B:114:PRO:HG2	1:B:115:GLN:HE21	1.81	0.46
1:B:353:VAL:HG13	1:B:370:PHE:CD1	2.51	0.46
2:C:185:VAL:CG1	2:C:186:VAL:N	2.79	0.46
2:C:5:GLU:OE1	2:C:5:GLU:HA	2.16	0.46
1:F:146:LEU:CD2	2:H:18:MET:HG3	2.46	0.46
1:F:151:GLU:O	1:F:155:ARG:HG3	2.16	0.46
2:H:123:GLN:NE2	2:H:126:ILE:HG13	2.30	0.46
1:A:154:VAL:O	1:A:158:LEU:HD12	2.17	0.45
2:D:11:ARG:O	2:D:15:GLY:N	2.44	0.45
2:D:86:ASN:OD1	2:D:88:LEU:HB2	2.15	0.45
2:G:115:ALA:O	2:G:118:LEU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:NH1	1:A:385:ARG:HG3	2.31	0.45
2:C:125:TYR:CD2	2:C:146:ARG:HB3	2.51	0.45
2:C:36:VAL:HG23	2:C:37:GLN:N	2.30	0.45
1:E:157:LEU:O	1:E:160:GLN:HB2	2.16	0.45
2:G:123:GLN:HA	2:G:126:ILE:HG13	1.99	0.45
2:C:17:GLY:O	2:C:18:MET:C	2.54	0.45
2:G:60:ILE:HD12	2:H:192:PHE:HB3	1.98	0.45
1:A:141:VAL:HG21	1:A:147:LEU:CD2	2.47	0.45
1:B:185:ASN:HB3	1:B:188:THR:OG1	2.16	0.45
1:B:289:LEU:HD23	1:B:289:LEU:H	1.81	0.45
2:C:46:LYS:H	2:C:46:LYS:HG2	1.44	0.45
2:G:122:ARG:O	2:G:125:TYR:N	2.50	0.45
1:E:263:ARG:NH2	1:E:297:GLU:HG2	2.32	0.45
1:F:19:HIS:O	1:F:22:HIS:HB2	2.16	0.45
2:G:130:LEU:HA	2:G:130:LEU:HD12	1.80	0.45
2:G:136:GLN:O	2:G:137:GLN:C	2.53	0.45
2:H:100:ILE:HG23	2:H:105:PRO:HD2	1.97	0.45
2:D:38:LEU:HD12	2:D:38:LEU:HA	1.78	0.45
1:E:198:LYS:O	1:E:201:GLU:HB2	2.15	0.45
1:E:385:ARG:CG	1:E:385:ARG:NH1	2.78	0.45
1:F:298:VAL:C	1:F:299:GLU:HG3	2.36	0.45
2:H:116:GLU:N	2:H:116:GLU:OE1	2.48	0.45
1:A:17:ILE:HD13	1:A:17:ILE:N	2.30	0.45
1:A:190:ARG:HD3	1:A:200:TRP:CG	2.52	0.45
1:B:176:LEU:O	1:B:180:GLU:HG3	2.17	0.45
2:D:131:ASN:C	2:D:133:GLY:H	2.16	0.45
2:D:130:LEU:CD1	2:D:135:PRO:HA	2.40	0.45
1:E:190:ARG:HD3	1:E:200:TRP:CG	2.52	0.45
1:E:267:VAL:HG12	1:E:269:GLY:H	1.82	0.45
2:G:121:GLU:O	2:G:122:ARG:C	2.54	0.45
2:H:7:ILE:HD11	2:H:22:LYS:HA	1.99	0.45
1:A:254:GLU:O	1:A:304:LEU:HA	2.16	0.45
1:A:310:ILE:HG12	1:A:311:THR:N	2.32	0.45
1:B:225:VAL:HG13	1:B:238:ALA:HB1	1.98	0.45
2:C:28:ALA:HB2	2:C:38:LEU:CD2	2.46	0.45
2:C:60:ILE:HD12	2:D:192:PHE:CB	2.47	0.45
1:E:385:ARG:HH11	1:E:385:ARG:HG3	1.80	0.45
1:F:293:VAL:HA	1:F:297:GLU:OE1	2.16	0.45
1:F:347:THR:OG1	1:F:348:ASP:N	2.48	0.45
2:H:6:LEU:O	2:H:25:LEU:HD11	2.17	0.45
1:A:222:LEU:HA	1:A:305:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ARG:HB3	1:A:393:ARG:HE	1.60	0.45
1:B:304:LEU:N	1:B:304:LEU:HD22	2.32	0.45
2:C:165:ASP:OD1	2:C:165:ASP:N	2.50	0.45
2:H:165:ASP:N	2:H:165:ASP:OD1	2.50	0.45
2:C:120:LYS:HG2	2:C:124:ILE:CD1	2.47	0.45
1:B:109:ALA:HA	2:D:19:MET:CG	2.46	0.45
2:D:81:ASP:C	2:D:81:ASP:OD1	2.56	0.45
1:A:156:ASP:HA	1:A:159:ASN:HD22	1.82	0.44
2:D:19:MET:HB3	2:D:23:ARG:CZ	2.46	0.44
1:F:299:GLU:H	1:F:302:GLN:HE21	1.65	0.44
2:H:81:ASP:OD1	2:H:81:ASP:C	2.56	0.44
2:H:94:LYS:HA	2:H:94:LYS:HD3	1.71	0.44
1:A:316:PHE:HA	1:A:404:LEU:HG	1.99	0.44
1:B:223:MET:O	1:B:303:VAL:HG22	2.17	0.44
1:A:318:ALA:HA	1:A:401:THR:HG23	1.99	0.44
1:B:15:GLY:HA3	1:B:99:MET:SD	2.57	0.44
1:B:210:ILE:HG22	1:B:210:ILE:O	2.17	0.44
2:C:94:LYS:HA	2:C:94:LYS:HD3	1.61	0.44
1:E:228:VAL:HG12	1:E:229:PHE:N	2.33	0.44
1:E:385:ARG:CB	1:E:385:ARG:HH11	2.29	0.44
2:G:135:PRO:O	2:G:138:ILE:HB	2.17	0.44
2:H:36:VAL:O	2:H:39:LEU:HB2	2.18	0.44
1:B:199:ILE:O	1:B:202:LEU:HB3	2.17	0.44
1:E:247:VAL:O	1:E:247:VAL:CG1	2.62	0.44
2:G:165:ASP:N	2:G:165:ASP:OD1	2.51	0.44
1:A:291:ARG:CB	1:A:291:ARG:NH1	2.80	0.44
1:B:111:GLY:HA2	1:B:150:VAL:HG13	1.99	0.44
2:C:135:PRO:HB2	2:C:137:GLN:HE22	1.82	0.44
2:D:119:GLU:C	2:D:121:GLU:H	2.21	0.44
1:E:221:PHE:CG	1:E:222:LEU:N	2.86	0.44
1:E:236:THR:HG1	1:E:293:VAL:HG23	1.83	0.44
1:E:272:MET:HB2	1:E:277:LEU:HD12	2.00	0.44
1:F:130:TYR:HE1	1:F:164:PRO:CG	2.30	0.44
2:H:7:ILE:HG12	2:H:25:LEU:HD13	1.99	0.44
2:H:38:LEU:HA	2:H:38:LEU:HD12	1.90	0.44
1:A:253:VAL:HG22	1:A:254:GLU:N	2.31	0.44
1:B:312:PRO:HA	1:B:378:VAL:O	2.18	0.44
1:B:342:PHE:N	1:B:342:PHE:HD1	2.16	0.44
2:C:120:LYS:HE2	2:C:124:ILE:HD11	1.99	0.44
2:G:172:LEU:HD12	2:G:172:LEU:O	2.17	0.44
1:A:265:THR:HG21	1:A:293:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NH2	1:B:170:VAL:HG23	2.33	0.44
1:B:216:ASP:O	1:B:218:ASP:N	2.51	0.44
1:B:223:MET:HE3	1:B:304:LEU:HD21	2.00	0.44
1:E:251:ASP:O	1:E:267:VAL:HG23	2.18	0.44
2:H:123:GLN:HE22	2:H:126:ILE:HG13	1.82	0.44
2:H:185:VAL:CG1	2:H:186:VAL:N	2.81	0.44
2:H:11:ARG:HD3	2:H:18:MET:SD	2.58	0.44
1:B:230:THR:HG22	1:B:235:GLY:O	2.18	0.44
1:B:295:ARG:NH1	1:B:295:ARG:CG	2.79	0.44
1:B:298:VAL:C	1:B:299:GLU:HG3	2.37	0.44
2:D:92:LEU:HD12	2:D:92:LEU:O	2.18	0.44
2:G:109:SER:HA	2:G:157:LEU:HD23	2.00	0.44
2:D:165:ASP:N	2:D:165:ASP:OD1	2.51	0.43
1:E:259:ALA:HB1	1:E:260:PRO:HD2	1.99	0.43
1:F:241:ARG:HG2	1:F:242:ILE:O	2.18	0.43
2:G:81:ASP:C	2:G:81:ASP:OD1	2.56	0.43
2:H:115:ALA:HA	2:H:118:LEU:HD12	1.99	0.43
1:A:188:THR:HG22	1:A:189:ARG:N	2.33	0.43
1:A:393:ARG:O	1:A:395:VAL:HG13	2.17	0.43
1:B:284:ASP:O	1:B:286:VAL:HG13	2.18	0.43
1:B:268:THR:HB	1:B:289:LEU:HD12	2.00	0.43
1:B:289:LEU:HD23	1:B:289:LEU:N	2.33	0.43
2:D:147:LEU:HA	2:D:147:LEU:HD23	1.81	0.43
2:D:2:SER:HB2	2:D:3:GLN:H	1.54	0.43
1:F:271:GLU:HG2	1:F:274:ARG:HA	2.00	0.43
1:F:291:ARG:HH11	1:F:291:ARG:HB2	1.80	0.43
2:H:86:ASN:OD1	2:H:88:LEU:HB2	2.17	0.43
1:A:12:VAL:HG13	1:A:100:ASP:HB2	1.99	0.43
2:D:27:ASP:CG	2:D:42:ARG:HH22	2.22	0.43
1:E:254:GLU:O	1:E:304:LEU:HA	2.19	0.43
1:F:393:ARG:HE	1:F:393:ARG:HB3	1.66	0.43
2:G:80:THR:HG23	2:G:182:GLU:OE2	2.18	0.43
2:H:67:ASN:OD1	2:H:67:ASN:C	2.56	0.43
2:G:90:GLN:HE22	2:H:68:GLN:HE22	1.65	0.43
1:A:115:GLN:HG2	2:C:83:VAL:HG23	2.00	0.43
1:B:264:ARG:HH11	1:B:264:ARG:CG	2.06	0.43
2:C:130:LEU:HD21	2:C:136:GLN:HA	1.99	0.43
2:C:168:LYS:O	2:C:171:GLU:HB2	2.18	0.43
2:D:62:HIS:HA	2:D:72:VAL:O	2.18	0.43
1:F:264:ARG:NH1	1:F:264:ARG:CG	2.76	0.43
1:B:169:PRO:HD3	1:B:209:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ILE:HG23	2:D:105:PRO:HD2	2.00	0.43
2:D:17:GLY:O	2:D:20:ASP:N	2.51	0.43
1:F:12:VAL:HG13	1:F:100:ASP:HB2	2.00	0.43
1:F:133:VAL:HG12	1:F:134:PHE:N	2.33	0.43
1:F:121:LEU:HG	1:F:161:TYR:CE2	2.53	0.43
1:F:265:THR:HG21	1:F:293:VAL:HG13	2.01	0.43
2:G:126:ILE:HD13	2:G:126:ILE:N	2.33	0.43
1:B:168:VAL:HG13	1:B:169:PRO:HD2	2.01	0.43
1:E:121:LEU:HG	1:E:161:TYR:CE2	2.53	0.43
1:E:265:THR:HG21	1:E:293:VAL:HG13	1.99	0.43
1:E:223:MET:HB3	1:E:304:LEU:CD2	2.48	0.43
1:F:182:MET:SD	1:F:188:THR:HB	2.59	0.43
1:A:237:VAL:CG1	1:A:238:ALA:N	2.81	0.43
2:C:74:VAL:HG13	2:C:74:VAL:O	2.19	0.43
1:E:237:VAL:CG1	1:E:238:ALA:N	2.81	0.43
1:E:312:PRO:HA	1:E:378:VAL:O	2.18	0.43
1:F:335:PHE:HA	1:F:355:LEU:HD11	2.00	0.43
2:H:8:LYS:HE2	2:H:9:LYS:HZ1	1.84	0.43
1:B:113:MET:O	1:B:116:THR:HB	2.18	0.43
1:B:146:LEU:CD2	2:D:19:MET:SD	3.07	0.43
1:F:275:LYS:O	1:F:276:THR:O	2.36	0.43
1:A:312:PRO:HA	1:A:378:VAL:O	2.19	0.43
1:B:136:ASN:CG	1:B:137:LYS:N	2.72	0.43
2:C:7:ILE:O	2:C:9:LYS:N	2.51	0.43
2:C:81:ASP:OD1	2:C:81:ASP:C	2.57	0.43
2:D:8:LYS:O	2:D:12:GLU:HB3	2.19	0.43
2:G:3:GLN:NE2	2:G:30:TRP:CE3	2.87	0.43
2:G:74:VAL:O	2:G:74:VAL:HG13	2.19	0.43
1:E:17:ILE:HD13	1:E:103:ILE:O	2.19	0.43
2:C:132:GLU:OE2	2:C:134:LYS:HE2	2.18	0.42
2:C:138:ILE:CG2	2:C:139:ALA:N	2.82	0.42
2:C:14:THR:HG21	2:C:40:ARG:HH12	1.82	0.42
2:D:4:MET:HA	2:D:7:ILE:HD12	1.99	0.42
1:F:265:THR:O	1:F:266:VAL:HG23	2.19	0.42
1:F:375:ILE:HG13	1:F:376:LYS:N	2.34	0.42
1:F:93:ILE:C	1:F:95:GLY:H	2.22	0.42
1:A:349:VAL:CG1	1:A:350:THR:N	2.81	0.42
1:A:385:ARG:NH1	1:A:385:ARG:CG	2.79	0.42
1:A:39:ASN:HA	1:A:40:PRO:HD2	1.49	0.42
1:B:151:GLU:O	1:B:155:ARG:HG3	2.19	0.42
2:D:135:PRO:HD2	2:D:138:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:32:GLU:O	2:G:33:GLU:C	2.56	0.42
1:B:93:ILE:C	1:B:95:GLY:H	2.23	0.42
1:E:237:VAL:HG12	1:E:238:ALA:N	2.32	0.42
1:E:326:GLU:C	1:E:328:GLY:H	2.22	0.42
1:F:368:VAL:CG1	1:F:369:THR:H	2.18	0.42
2:H:84:ALA:HA	2:H:89:PHE:CD2	2.54	0.42
1:A:214:VAL:HG12	1:A:218:ASP:HB2	2.01	0.42
1:A:271:GLU:HG2	1:A:274:ARG:HA	2.02	0.42
1:A:311:THR:OG1	1:A:313:HIS:CE1	2.72	0.42
2:C:121:GLU:O	2:C:124:ILE:HB	2.19	0.42
2:D:7:ILE:HG23	2:D:21:VAL:CG1	2.49	0.42
1:F:85:HIS:O	1:F:89:ILE:HG12	2.19	0.42
2:G:126:ILE:HA	2:G:139:ALA:HB1	2.01	0.42
2:G:132:GLU:OE1	2:G:134:LYS:NZ	2.44	0.42
2:G:146:ARG:HH11	2:G:146:ARG:CG	2.17	0.42
1:A:231:ILE:O	1:A:232:THR:C	2.57	0.42
1:A:267:VAL:HG12	1:A:269:GLY:H	1.84	0.42
1:B:361:MET:CE	2:C:102:MET:HB2	2.49	0.42
2:C:92:LEU:HD11	2:C:96:LEU:HD11	2.01	0.42
1:E:100:ASP:O	1:E:129:PRO:HG2	2.20	0.42
1:E:393:ARG:HE	1:E:393:ARG:HB3	1.60	0.42
1:F:136:ASN:CG	1:F:137:LYS:N	2.73	0.42
2:G:35:ALA:O	2:G:36:VAL:C	2.58	0.42
2:H:109:SER:HB2	2:H:111:GLU:OE2	2.19	0.42
1:A:193:ASN:OD1	1:A:196:VAL:HG23	2.19	0.42
1:B:154:VAL:O	1:B:155:ARG:C	2.58	0.42
1:B:130:TYR:CE1	1:B:164:PRO:CG	3.01	0.42
2:D:53:ARG:HG2	2:D:79:GLU:CD	2.40	0.42
1:E:154:VAL:O	1:E:158:LEU:HD12	2.20	0.42
2:H:135:PRO:HB2	2:H:136:GLN:H	1.73	0.42
1:B:12:VAL:CG1	1:B:13:ASN:N	2.83	0.42
1:B:188:THR:HG22	1:B:189:ARG:N	2.35	0.42
1:B:271:GLU:HG3	1:B:275:LYS:H	1.84	0.42
1:F:138:VAL:O	1:F:141:VAL:HG13	2.20	0.42
2:G:194:LEU:CD2	2:H:58:GLY:O	2.67	0.42
2:G:42:ARG:HA	2:G:45:MET:CE	2.49	0.42
2:G:53:ARG:HG2	2:G:53:ARG:H	1.57	0.42
1:A:237:VAL:CG2	1:A:289:LEU:HB3	2.44	0.42
2:C:185:VAL:HG12	2:C:186:VAL:N	2.35	0.42
1:B:115:GLN:CG	2:D:83:VAL:HG22	2.47	0.42
1:F:117:ARG:HG3	1:F:161:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:THR:CG2	1:F:79:HIS:HE1	2.31	0.42
2:G:109:SER:HB2	2:G:111:GLU:OE2	2.20	0.42
2:H:79:GLU:HB2	2:H:182:GLU:OE1	2.20	0.42
1:A:237:VAL:HG12	1:A:238:ALA:N	2.34	0.42
1:B:12:VAL:HG22	1:B:213:PRO:CD	2.50	0.42
1:B:223:MET:O	1:B:304:LEU:HD23	2.19	0.42
1:B:268:THR:HG1	1:B:291:ARG:HG3	1.81	0.42
1:E:304:LEU:HD23	1:E:304:LEU:H	1.82	0.42
1:F:147:LEU:HD23	1:F:147:LEU:N	2.35	0.42
2:G:92:LEU:HD11	2:G:96:LEU:HD11	2.02	0.42
2:H:80:THR:HG23	2:H:182:GLU:OE2	2.20	0.42
1:B:85:HIS:O	1:B:89:ILE:HB	2.20	0.42
2:D:148:LYS:O	2:D:152:GLU:CG	2.68	0.42
2:D:78:CYS:SG	2:D:83:VAL:HG12	2.60	0.42
1:E:143:ASP:HA	1:E:144:PRO:HD3	1.78	0.42
1:F:326:GLU:C	1:F:328:GLY:N	2.72	0.42
1:F:81:ASP:O	1:F:83:PRO:HD3	2.20	0.42
2:G:6:LEU:HD23	2:G:25:LEU:HD22	2.02	0.42
1:A:199:ILE:O	1:A:202:LEU:HB3	2.20	0.41
1:B:168:VAL:CG2	1:B:209:TYR:OH	2.68	0.41
2:C:118:LEU:HD12	2:C:118:LEU:C	2.39	0.41
2:C:120:LYS:HB3	2:C:120:LYS:NZ	2.35	0.41
2:D:110:ALA:O	2:D:113:ILE:HG13	2.20	0.41
1:E:268:THR:HG22	1:E:268:THR:O	2.20	0.41
1:E:295:ARG:NH1	1:E:295:ARG:HG3	2.34	0.41
1:E:304:LEU:HD23	1:E:304:LEU:O	2.20	0.41
1:E:69:GLU:HG2	1:E:76:HIS:NE2	2.35	0.41
1:B:343:TYR:HE1	1:B:345:ARG:O	2.03	0.41
2:C:11:ARG:NE	2:C:16:ALA:O	2.53	0.41
1:E:12:VAL:HG13	1:E:100:ASP:HB2	2.02	0.41
1:E:130:TYR:CD2	1:E:209:TYR:HB3	2.55	0.41
1:E:188:THR:HG22	1:E:189:ARG:N	2.35	0.41
1:E:231:ILE:O	1:E:232:THR:C	2.57	0.41
1:A:80:VAL:HG12	1:A:81:ASP:H	1.85	0.41
1:B:12:VAL:HG13	1:B:100:ASP:HB2	2.01	0.41
2:C:180:ILE:HG22	2:C:182:GLU:N	2.36	0.41
2:D:185:VAL:CG1	2:D:186:VAL:N	2.83	0.41
1:E:81:ASP:O	1:E:83:PRO:HD3	2.19	0.41
1:F:289:LEU:HD23	1:F:289:LEU:N	2.35	0.41
2:G:19:MET:HB3	2:G:23:ARG:CZ	2.50	0.41
1:B:86:ALA:HA	1:B:89:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3:GLN:HA	2:C:6:LEU:HD12	2.03	0.41
2:D:84:ALA:HA	2:D:89:PHE:CD2	2.55	0.41
1:E:141:VAL:CG2	1:E:147:LEU:HD21	2.49	0.41
1:A:311:THR:OG1	1:A:313:HIS:HE1	2.04	0.41
2:D:114:PRO:HG2	2:D:117:GLU:CB	2.50	0.41
2:C:58:GLY:O	2:D:194:LEU:CD2	2.68	0.41
1:F:111:GLY:HA2	1:F:150:VAL:HG13	2.01	0.41
2:G:159:GLN:O	2:G:169:VAL:HG23	2.20	0.41
1:A:221:PHE:HA	1:A:245:GLY:HA3	2.02	0.41
1:A:281:ILE:O	1:A:282:ALA:C	2.59	0.41
1:B:299:GLU:H	1:B:302:GLN:HE21	1.68	0.41
2:C:109:SER:HB2	2:C:111:GLU:OE2	2.20	0.41
2:C:11:ARG:O	2:C:15:GLY:N	2.53	0.41
2:C:7:ILE:H	2:C:7:ILE:HG12	1.35	0.41
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.86	0.41
1:B:216:ASP:C	1:B:218:ASP:N	2.74	0.41
1:B:222:LEU:HA	1:B:305:ALA:HB2	2.02	0.41
2:C:147:LEU:HD23	2:C:147:LEU:HA	1.72	0.41
2:D:120:LYS:O	2:D:124:ILE:CD1	2.69	0.41
2:D:53:ARG:NH1	2:D:53:ARG:HG2	2.36	0.41
1:E:80:VAL:HG12	1:E:81:ASP:H	1.86	0.41
1:A:223:MET:HE1	1:A:304:LEU:HD21	2.01	0.41
1:A:228:VAL:HG12	1:A:229:PHE:N	2.36	0.41
1:A:268:THR:HG22	1:A:268:THR:O	2.21	0.41
1:A:272:MET:HB2	1:A:277:LEU:HD12	2.01	0.41
1:A:305:ALA:O	1:A:306:LYS:C	2.59	0.41
1:B:223:MET:O	1:B:303:VAL:CG2	2.68	0.41
1:B:295:ARG:HD3	1:B:295:ARG:C	2.41	0.41
1:F:291:ARG:CZ	1:F:291:ARG:CB	2.98	0.41
2:G:4:MET:O	2:G:5:GLU:C	2.59	0.41
2:H:148:LYS:O	2:H:152:GLU:CG	2.69	0.41
1:A:115:GLN:HG2	2:C:83:VAL:HG22	2.02	0.41
1:B:304:LEU:H	1:B:304:LEU:HD23	1.85	0.41
2:D:94:LYS:HD3	2:D:94:LYS:HA	1.72	0.41
1:F:210:ILE:O	1:F:211:PRO:C	2.56	0.41
2:G:92:LEU:HD12	2:G:92:LEU:O	2.21	0.41
1:A:130:TYR:HB3	1:A:209:TYR:HE2	1.82	0.41
1:E:310:ILE:HG12	1:E:311:THR:N	2.36	0.41
1:F:270:VAL:O	1:F:271:GLU:HB2	2.21	0.41
2:H:92:LEU:HD11	2:H:96:LEU:HD11	2.03	0.41
1:A:110:ASP:O	2:C:11:ARG:NH2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:HIS:CD2	1:A:76:HIS:CD2	3.08	0.41
1:A:304:LEU:O	1:A:304:LEU:HD23	2.21	0.41
1:A:93:ILE:C	1:A:95:GLY:N	2.74	0.41
1:B:149:LEU:HD22	2:D:4:MET:HB2	2.03	0.41
1:B:89:ILE:HA	1:B:89:ILE:HD12	1.77	0.41
1:E:136:ASN:CG	1:E:137:LYS:N	2.74	0.41
1:F:143:ASP:CG	1:F:145:GLU:HB2	2.41	0.41
1:F:297:GLU:O	1:F:298:VAL:HG23	2.21	0.41
1:B:95:GLY:H	1:B:385:ARG:HE	1.59	0.40
1:B:81:ASP:O	1:B:83:PRO:HD3	2.22	0.40
2:G:192:PHE:HB3	2:H:60:ILE:CD1	2.49	0.40
2:H:194:LEU:HD12	2:H:194:LEU:HA	1.82	0.40
1:A:18:GLY:HA2	1:A:119:HIS:CD2	2.56	0.40
1:E:130:TYR:HE1	1:E:164:PRO:HG2	1.87	0.40
1:E:316:PHE:HA	1:E:404:LEU:HG	2.03	0.40
1:E:93:ILE:C	1:E:95:GLY:N	2.74	0.40
1:B:117:ARG:HG3	1:B:161:TYR:OH	2.21	0.40
1:B:216:ASP:HA	1:B:219:LYS:CD	2.50	0.40
2:D:133:GLY:O	2:D:134:LYS:C	2.60	0.40
1:E:221:PHE:HA	1:E:245:GLY:HA3	2.03	0.40
1:E:222:LEU:HA	1:E:305:ALA:HB2	2.02	0.40
1:F:254:GLU:HG2	1:F:262:THR:HG22	2.03	0.40
1:A:259:ALA:HB1	1:A:260:PRO:HD2	2.02	0.40
1:A:298:VAL:C	1:A:299:GLU:HG3	2.41	0.40
2:C:192:PHE:CB	2:D:60:ILE:HD12	2.50	0.40
2:D:35:ALA:O	2:D:38:LEU:N	2.53	0.40
1:E:304:LEU:HD22	1:E:304:LEU:N	2.36	0.40
1:F:143:ASP:HA	1:F:144:PRO:HD3	1.81	0.40
1:F:115:GLN:CG	2:H:83:VAL:HG22	2.48	0.40
1:B:221:PHE:HE1	1:B:242:ILE:HG23	1.86	0.40
2:D:134:LYS:CB	2:D:138:ILE:HD12	2.48	0.40
2:D:70:VAL:HA	2:D:192:PHE:O	2.22	0.40
2:D:28:ALA:HB2	2:D:38:LEU:HD22	2.02	0.40
1:E:291:ARG:CB	1:E:291:ARG:NH1	2.83	0.40
2:G:180:ILE:HG22	2:G:182:GLU:N	2.37	0.40
2:G:185:VAL:CG1	2:G:186:VAL:N	2.85	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	369/405 (91%)	327 (89%)	34 (9%)	8 (2%)	8	36
1	B	369/405 (91%)	308 (84%)	46 (12%)	15 (4%)	3	19
1	E	368/405 (91%)	319 (87%)	39 (11%)	10 (3%)	6	30
1	F	368/405 (91%)	308 (84%)	46 (12%)	14 (4%)	4	21
2	C	193/196 (98%)	164 (85%)	20 (10%)	9 (5%)	3	16
2	D	193/196 (98%)	161 (83%)	25 (13%)	7 (4%)	4	22
2	G	193/196 (98%)	162 (84%)	20 (10%)	11 (6%)	2	12
2	H	192/196 (98%)	165 (86%)	20 (10%)	7 (4%)	4	22
All	All	2245/2404 (93%)	1914 (85%)	250 (11%)	81 (4%)	4	22

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	THR
1	B	67	HIS
1	B	232	THR
1	B	276	THR
2	C	29	GLY
2	D	132	GLU
1	E	276	THR
1	F	232	THR
1	F	276	THR
2	G	29	GLY
2	G	32	GLU
2	G	136	GLN
2	G	137	GLN
2	H	29	GLY
2	H	134	LYS
1	A	95	GLY
1	B	96	ALA

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Mol	Chain	Res	Type
2	C	5	GLU
2	C	8	LYS
2	C	27	ASP
2	C	30	TRP
2	C	32	GLU
2	C	33	GLU
2	D	27	ASP
2	D	29	GLY
1	E	95	GLY
1	E	247	VAL
1	F	309	SER
2	G	51	ALA
2	H	32	GLU
2	H	135	PRO
1	A	96	ALA
1	A	247	VAL
1	A	345	ARG
1	B	208	GLU
1	B	340	PRO
1	B	345	ARG
2	C	35	ALA
2	D	135	PRO
1	E	345	ARG
1	F	96	ALA
1	F	98	GLN
1	F	220	PRO
1	F	300	ARG
1	F	345	ARG
2	G	30	TRP
2	G	33	GLU
2	G	127	GLN
2	H	51	ALA
1	A	232	THR
1	B	330	ARG
2	C	4	MET
1	E	37	ALA
1	E	96	ALA
1	E	232	THR
1	F	222	LEU
1	F	330	ARG
1	F	340	PRO
2	G	27	ASP

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Mol	Chain	Res	Type
2	H	131	ASN
1	B	215	ARG
2	D	51	ALA
2	D	116	GLU
2	D	164	ASP
1	B	95	GLY
1	B	98	GLN
1	E	98	GLN
1	E	340	PRO
1	F	95	GLY
2	G	8	LYS
2	H	27	ASP
1	B	217	VAL
1	E	392	GLY
1	F	247	VAL
1	A	392	GLY
1	B	213	PRO
1	F	10	PRO
2	G	138	ILE
1	A	340	PRO
1	B	10	PRO
1	B	247	VAL

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	306/339 (90%)	266 (87%)	40 (13%)	5	21
1	B	306/339 (90%)	256 (84%)	50 (16%)	3	13
1	E	308/339 (91%)	270 (88%)	38 (12%)	5	24
1	F	302/339 (89%)	254 (84%)	48 (16%)	3	14
2	C	157/162 (97%)	121 (77%)	36 (23%)	1	5
2	D	150/162 (93%)	119 (79%)	31 (21%)	1	6
2	G	157/162 (97%)	129 (82%)	28 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	152/162 (94%)	118 (78%)	34 (22%)	1 5
All	All	1838/2004 (92%)	1533 (83%)	305 (17%)	2 13

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	20	VAL
1	A	32	THR
1	A	69	GLU
1	A	79	HIS
1	A	98	GLN
1	A	115	GLN
1	A	121	LEU
1	A	124	ARG
1	A	126	VAL
1	A	138	VAL
1	A	141	VAL
1	A	142	ASP
1	A	155	ARG
1	A	158	LEU
1	A	166	ASP
1	A	231	ILE
1	A	239	THR
1	A	248	LYS
1	A	263	ARG
1	A	264	ARG
1	A	277	LEU
1	A	278	GLN
1	A	289	LEU
1	A	290	LEU
1	A	295	ARG
1	A	299	GLU
1	A	304	LEU
1	A	332	THR
1	A	339	ARG
1	A	341	GLN
1	A	343	TYR
1	A	347	THR
1	A	348	ASP
1	A	352	VAL
1	A	367	ASN

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Mol	Chain	Res	Type
1	A	374	LEU
1	A	382	GLU
1	A	385	ARG
1	A	393	ARG
1	B	17	ILE
1	B	20	VAL
1	B	32	THR
1	B	65	THR
1	B	69	GLU
1	B	98	GLN
1	B	115	GLN
1	B	126	VAL
1	B	130	TYR
1	B	138	VAL
1	B	141	VAL
1	B	142	ASP
1	B	146	LEU
1	B	152	MET
1	B	155	ARG
1	B	166	ASP
1	B	176	LEU
1	B	210	ILE
1	B	212	THR
1	B	215	ARG
1	B	229	PHE
1	B	230	THR
1	B	232	THR
1	B	239	THR
1	B	248	LYS
1	B	252	GLU
1	B	263	ARG
1	B	264	ARG
1	B	277	LEU
1	B	278	GLN
1	B	289	LEU
1	B	290	LEU
1	B	295	ARG
1	B	299	GLU
1	B	302	GLN
1	B	303	VAL
1	B	304	LEU
1	B	309	SER

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Mol	Chain	Res	Type
1	B	332	THR
1	B	339	ARG
1	B	342	PHE
1	B	343	TYR
1	B	347	THR
1	B	348	ASP
1	B	352	VAL
1	B	367	ASN
1	B	374	LEU
1	B	382	GLU
1	B	385	ARG
1	B	405	GLU
2	C	3	GLN
2	C	4	MET
2	C	5	GLU
2	C	6	LEU
2	C	7	ILE
2	C	8	LYS
2	C	10	LEU
2	C	11	ARG
2	C	18	MET
2	C	23	ARG
2	C	27	ASP
2	C	33	GLU
2	C	34	LYS
2	C	37	GLN
2	C	40	ARG
2	C	50	LYS
2	C	53	ARG
2	C	94	LYS
2	C	103	MET
2	C	117	GLU
2	C	119	GLU
2	C	120	LYS
2	C	121	GLU
2	C	122	ARG
2	C	123	GLN
2	C	127	GLN
2	C	134	LYS
2	C	137	GLN
2	C	138	ILE
2	C	141	LYS

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Mol	Chain	Res	Type
2	C	157	LEU
2	C	162	VAL
2	C	167	VAL
2	C	175	GLN
2	C	179	LYS
2	C	180	ILE
2	D	2	SER
2	D	3	GLN
2	D	4	MET
2	D	5	GLU
2	D	14	THR
2	D	23	ARG
2	D	27	ASP
2	D	31	ASP
2	D	33	GLU
2	D	37	GLN
2	D	50	LYS
2	D	56	ARG
2	D	94	LYS
2	D	103	MET
2	D	116	GLU
2	D	117	GLU
2	D	118	LEU
2	D	119	GLU
2	D	122	ARG
2	D	123	GLN
2	D	125	TYR
2	D	130	LEU
2	D	132	GLU
2	D	134	LYS
2	D	141	LYS
2	D	157	LEU
2	D	162	VAL
2	D	167	VAL
2	D	175	GLN
2	D	179	LYS
2	D	180	ILE
1	E	17	ILE
1	E	20	VAL
1	E	32	THR
1	E	69	GLU
1	E	79	HIS

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Mol	Chain	Res	Type
1	E	98	GLN
1	E	115	GLN
1	E	121	LEU
1	E	126	VAL
1	E	138	VAL
1	E	141	VAL
1	E	142	ASP
1	E	155	ARG
1	E	158	LEU
1	E	215	ARG
1	E	231	ILE
1	E	239	THR
1	E	248	LYS
1	E	263	ARG
1	E	264	ARG
1	E	277	LEU
1	E	278	GLN
1	E	289	LEU
1	E	290	LEU
1	E	295	ARG
1	E	299	GLU
1	E	303	VAL
1	E	304	LEU
1	E	332	THR
1	E	339	ARG
1	E	347	THR
1	E	352	VAL
1	E	367	ASN
1	E	374	LEU
1	E	382	GLU
1	E	385	ARG
1	E	393	ARG
1	E	405	GLU
1	F	17	ILE
1	F	20	VAL
1	F	24	LYS
1	F	32	THR
1	F	69	GLU
1	F	79	HIS
1	F	115	GLN
1	F	126	VAL
1	F	138	VAL

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Mol	Chain	Res	Type
1	F	141	VAL
1	F	142	ASP
1	F	146	LEU
1	F	152	MET
1	F	155	ARG
1	F	158	LEU
1	F	166	ASP
1	F	189	ARG
1	F	212	THR
1	F	215	ARG
1	F	217	VAL
1	F	223	MET
1	F	229	PHE
1	F	230	THR
1	F	232	THR
1	F	239	THR
1	F	244	ARG
1	F	248	LYS
1	F	252	GLU
1	F	264	ARG
1	F	289	LEU
1	F	295	ARG
1	F	299	GLU
1	F	302	GLN
1	F	303	VAL
1	F	311	THR
1	F	332	THR
1	F	339	ARG
1	F	342	PHE
1	F	343	TYR
1	F	347	THR
1	F	348	ASP
1	F	352	VAL
1	F	361	MET
1	F	367	ASN
1	F	374	LEU
1	F	382	GLU
1	F	385	ARG
1	F	393	ARG
2	G	3	GLN
2	G	5	GLU
2	G	8	LYS

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Mol	Chain	Res	Type
2	G	10	LEU
2	G	14	THR
2	G	23	ARG
2	G	31	ASP
2	G	34	LYS
2	G	37	GLN
2	G	50	LYS
2	G	56	ARG
2	G	94	LYS
2	G	103	MET
2	G	120	LYS
2	G	126	ILE
2	G	130	LEU
2	G	134	LYS
2	G	137	GLN
2	G	138	ILE
2	G	140	GLU
2	G	141	LYS
2	G	146	ARG
2	G	157	LEU
2	G	162	VAL
2	G	167	VAL
2	G	175	GLN
2	G	179	LYS
2	G	180	ILE
2	H	3	GLN
2	H	5	GLU
2	H	8	LYS
2	H	10	LEU
2	H	23	ARG
2	H	33	GLU
2	H	37	GLN
2	H	41	GLU
2	H	46	LYS
2	H	50	LYS
2	H	56	ARG
2	H	94	LYS
2	H	103	MET
2	H	106	ARG
2	H	117	GLU
2	H	118	LEU
2	H	119	GLU

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Mol	Chain	Res	Type
2	H	122	ARG
2	H	123	GLN
2	H	126	ILE
2	H	127	GLN
2	H	131	ASN
2	H	132	GLU
2	H	134	LYS
2	H	136	GLN
2	H	141	LYS
2	H	142	ILE
2	H	146	ARG
2	H	157	LEU
2	H	162	VAL
2	H	167	VAL
2	H	175	GLN
2	H	179	LYS
2	H	180	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	13	ASN
1	A	79	HIS
1	A	91	ASN
1	A	98	GLN
1	A	115	GLN
1	A	119	HIS
1	A	159	ASN
1	A	302	GLN
1	A	313	HIS
1	A	367	ASN
1	B	11	HIS
1	B	13	ASN
1	B	98	GLN
1	B	115	GLN
1	B	159	ASN
1	B	302	GLN
1	B	313	HIS
2	C	3	GLN
2	C	90	GLN
2	C	99	HIS

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Mol	Chain	Res	Type
2	C	137	GLN
2	C	183	ASN
2	D	90	GLN
2	D	99	HIS
2	D	131	ASN
2	D	183	ASN
1	E	11	HIS
1	E	13	ASN
1	E	79	HIS
1	E	91	ASN
1	E	98	GLN
1	E	115	GLN
1	E	119	HIS
1	E	302	GLN
1	E	313	HIS
1	E	341	GLN
1	E	367	ASN
1	F	11	HIS
1	F	79	HIS
1	F	115	GLN
1	F	159	ASN
1	F	302	GLN
1	F	313	HIS
1	F	341	GLN
1	F	367	ASN
2	G	3	GLN
2	G	90	GLN
2	G	99	HIS
2	H	90	GLN
2	H	99	HIS
2	H	123	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	373/405 (92%)	-0.74	1 (0%) 93 82	25, 50, 91, 109	0
1	B	373/405 (92%)	-0.45	2 (0%) 90 74	45, 94, 109, 110	0
1	E	372/405 (91%)	-0.75	0 100 100	20, 46, 84, 110	0
1	F	372/405 (91%)	-0.23	9 (2%) 59 30	34, 96, 110, 110	0
2	C	195/196 (99%)	-0.81	0 100 100	23, 60, 90, 100	0
2	D	195/196 (99%)	-0.69	0 100 100	31, 75, 109, 110	0
2	G	195/196 (99%)	-0.80	0 100 100	18, 49, 91, 104	0
2	H	194/196 (98%)	-0.67	0 100 100	23, 76, 109, 110	0
All	All	2269/2404 (94%)	-0.61	12 (0%) 90 74	18, 67, 109, 110	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	253	VAL	6.5
1	F	66	ALA	5.4
1	B	253	VAL	4.8
1	F	262	THR	3.4
1	B	65	THR	2.4
1	F	380	LEU	2.3
1	F	269	GLY	2.3
1	F	264	ARG	2.1
1	F	256	VAL	2.1
1	F	67	HIS	2.1
1	F	254	GLU	2.1
1	A	66	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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.