



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 04:35 PM EDT

PDB ID : 1K32
Title : Crystal structure of the tricorn protease
Authors : Brandstetter, H.; Kim, J.-S.; Groll, M.; Huber, R.
Deposited on : 2001-10-01
Resolution : 2.00 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

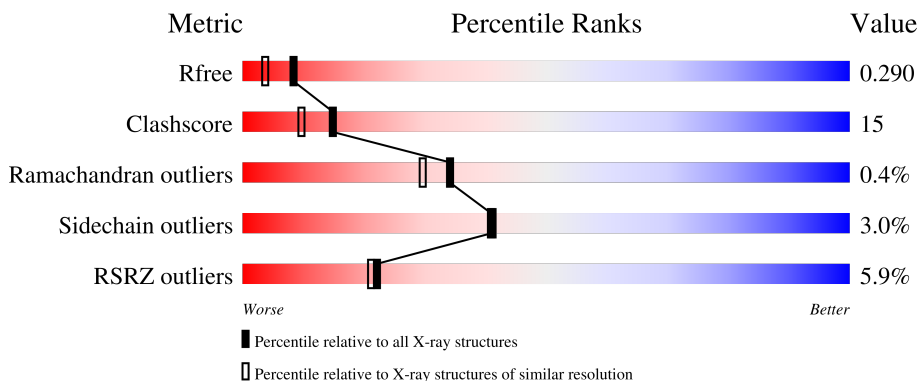
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


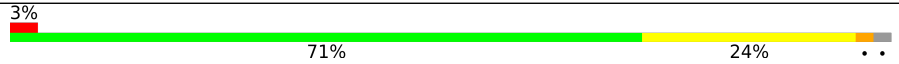
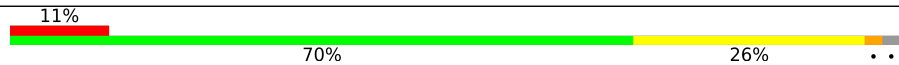

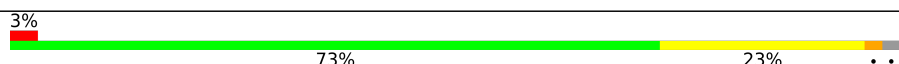
The reported resolution of this entry is 2.00 Å.

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	1045	 3% 72% 23% ..
1	B	1045	 3% 71% 24% ..
1	C	1045	 11% 70% 26% ..
1	D	1045	 4% 73% 23% ..
1	E	1045	 3% 73% 23% ..

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Mol	Chain	Length	Quality of chain
1	F	1045	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a red segment on the left labeled '10%', a green segment in the middle labeled '67%', and a yellow segment on the right labeled '23%'. The total length of the bar represents 100%. There are two small black dots at the far right end of the bar.</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 51456 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 tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1023	8177	5196	1402	1551	28	95	0	0
1	B	1023	8177	5196	1402	1551	28	95	0	0
1	C	1023	8177	5196	1402	1551	28	95	0	0
1	D	1023	8177	5196	1402	1551	28	95	0	0
1	E	1023	8177	5196	1402	1551	28	95	0	0
1	F	1023	8177	5196	1402	1551	28	95	0	0

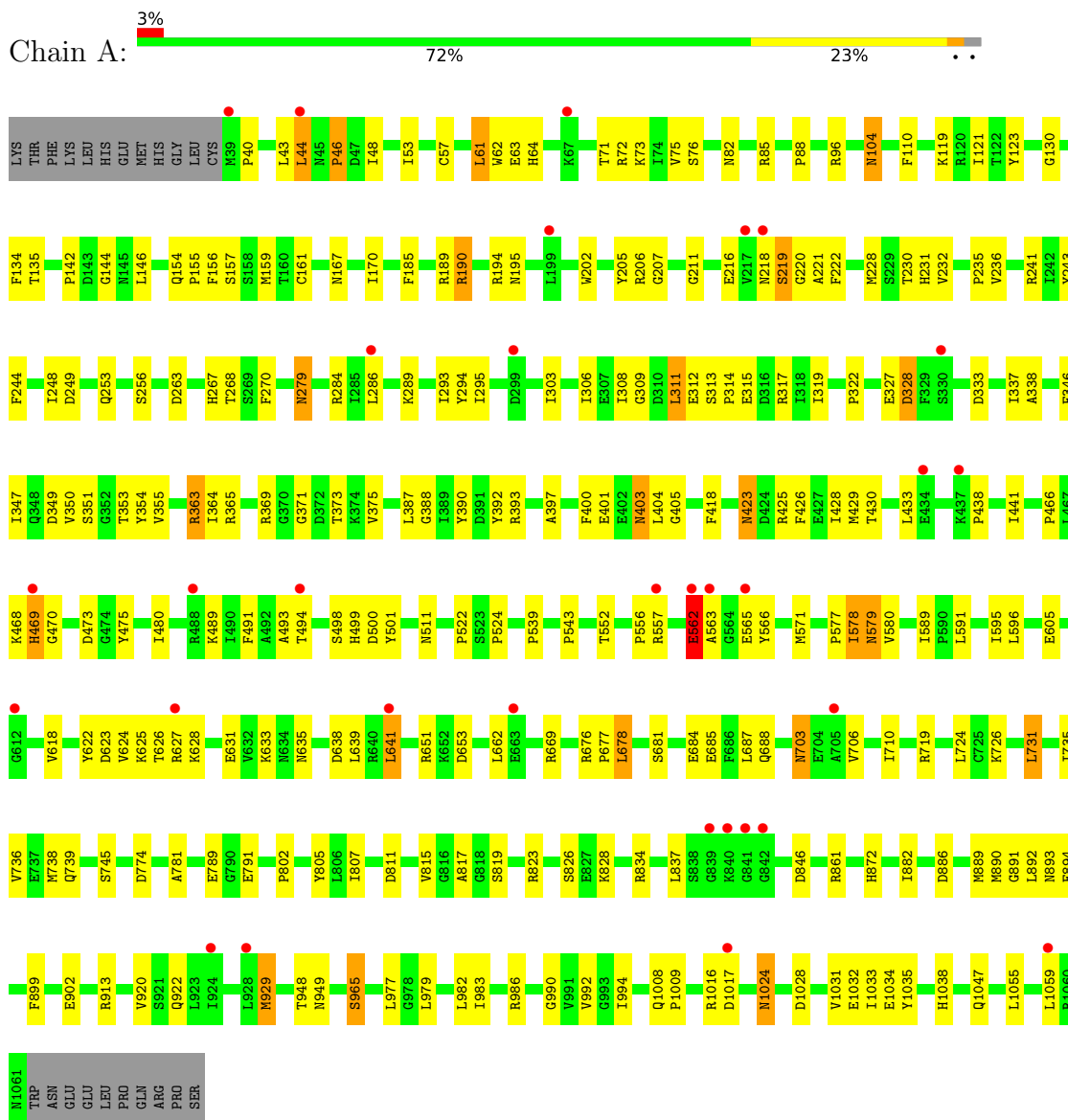
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	401	Total 401	O 401	0	0
2	B	395	Total 395	O 395	0	0
2	C	398	Total 398	O 398	0	0
2	D	401	Total 401	O 401	0	0
2	E	405	Total 405	O 405	0	0
2	F	394	Total 394	O 394	0	0

3 Residue-property plots [i](#)

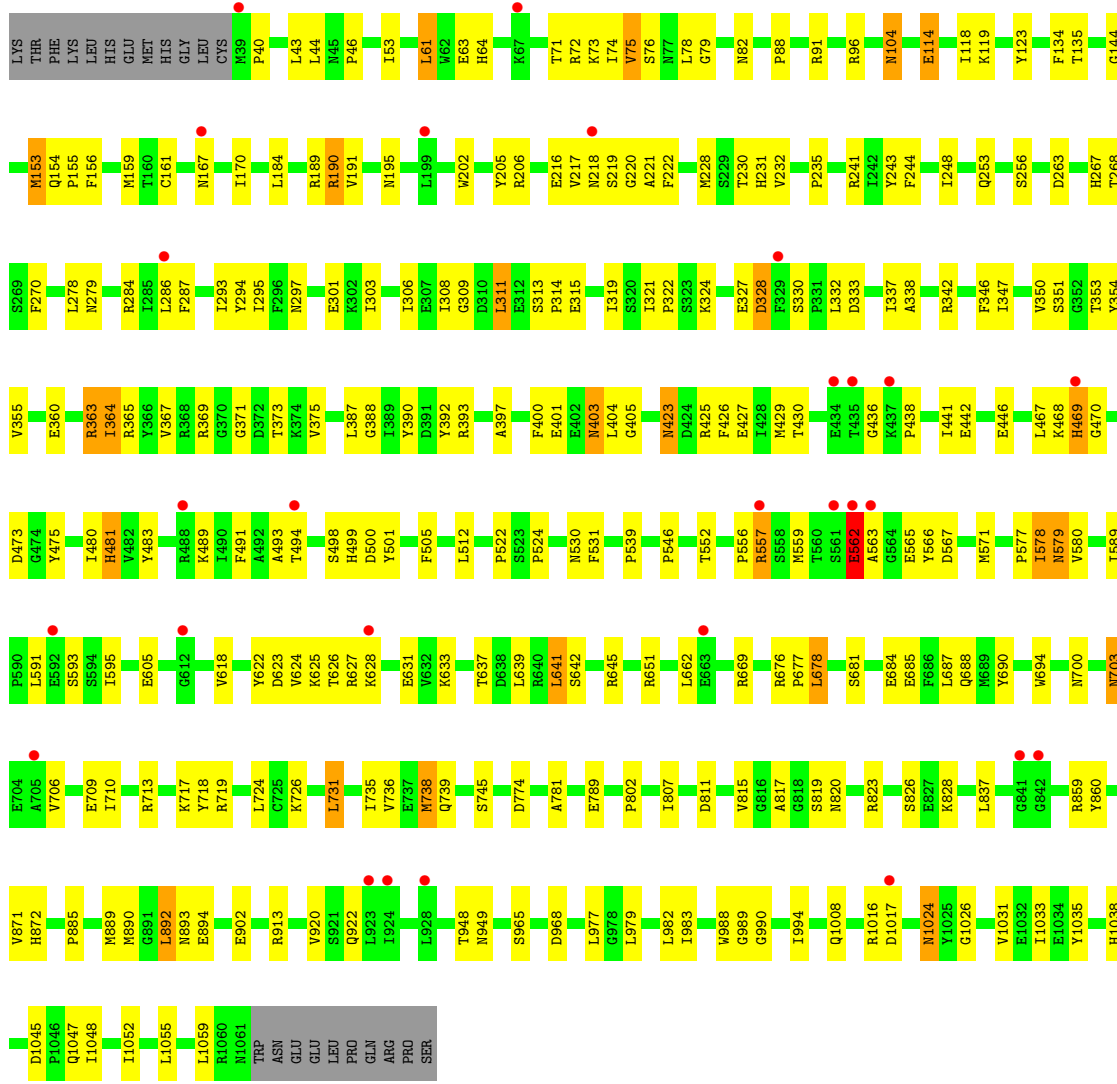
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: tricorn protease

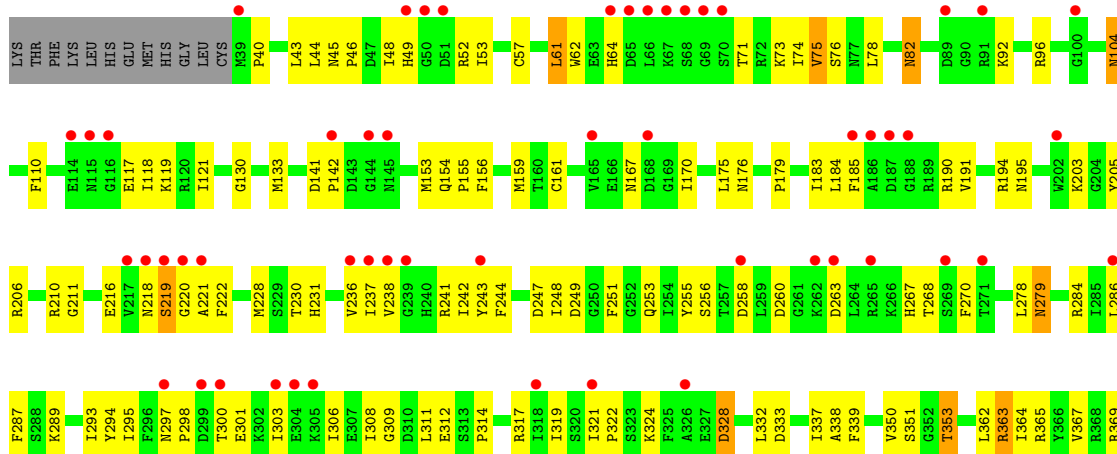


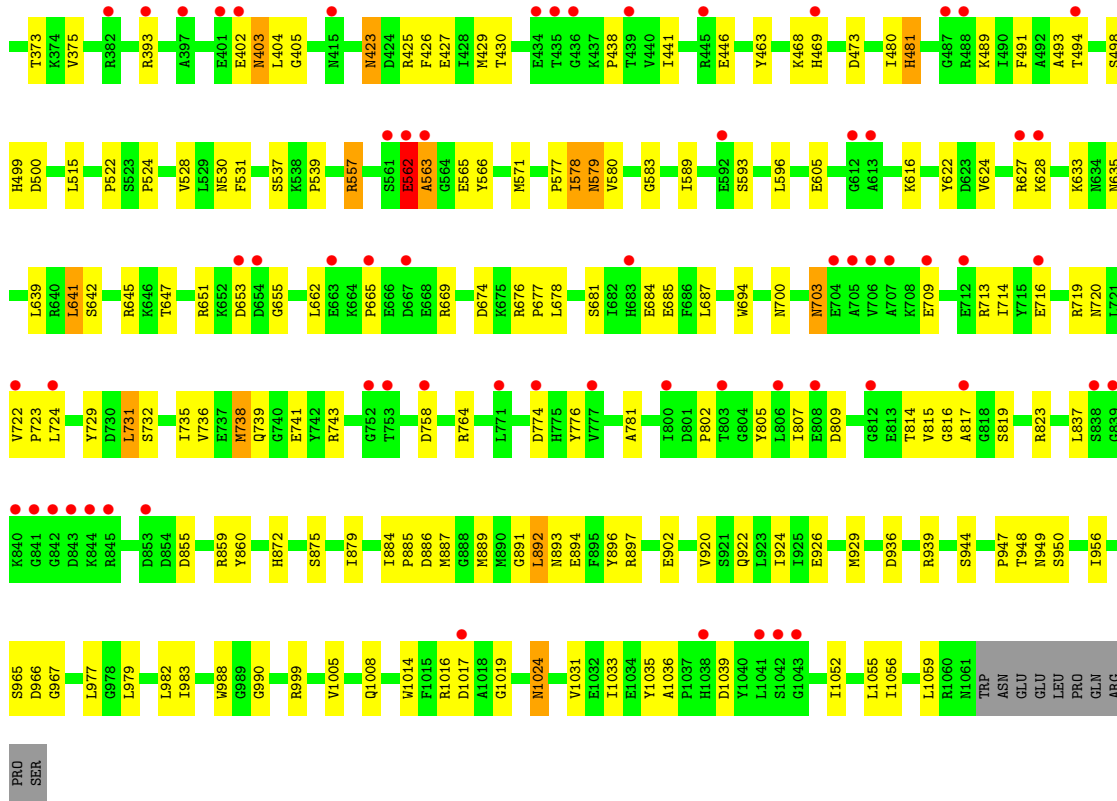
- Molecule 1: tricorn protease



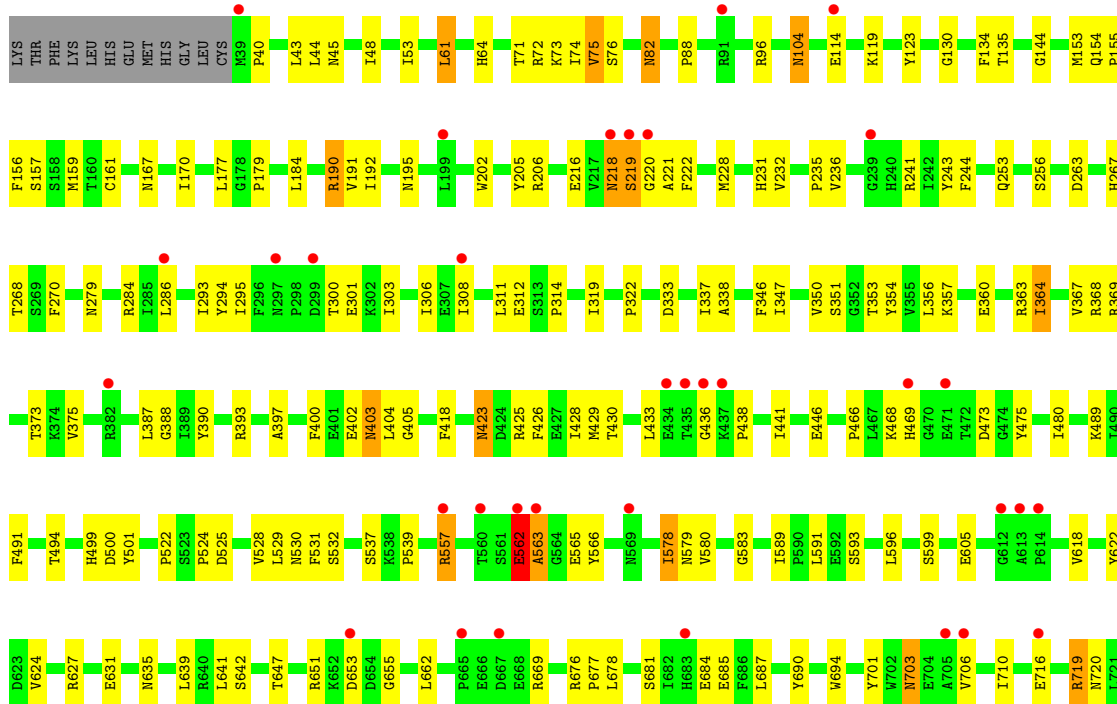
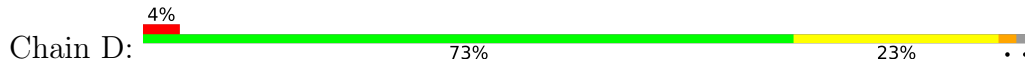


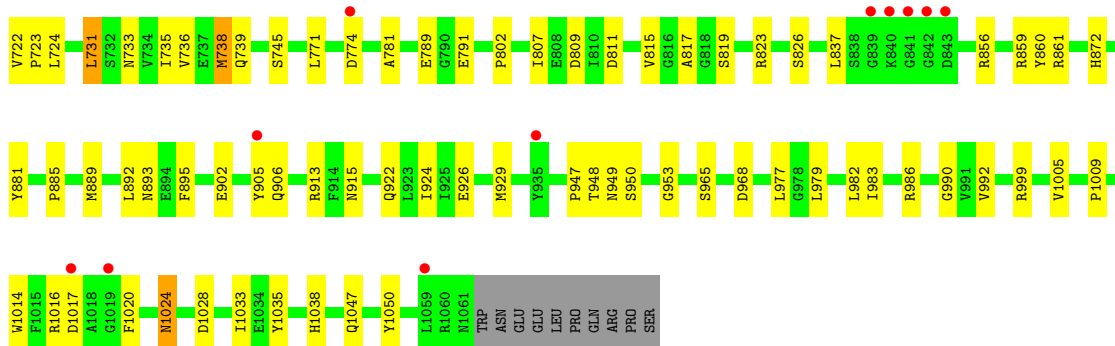
● Molecule 1: tricorin protease



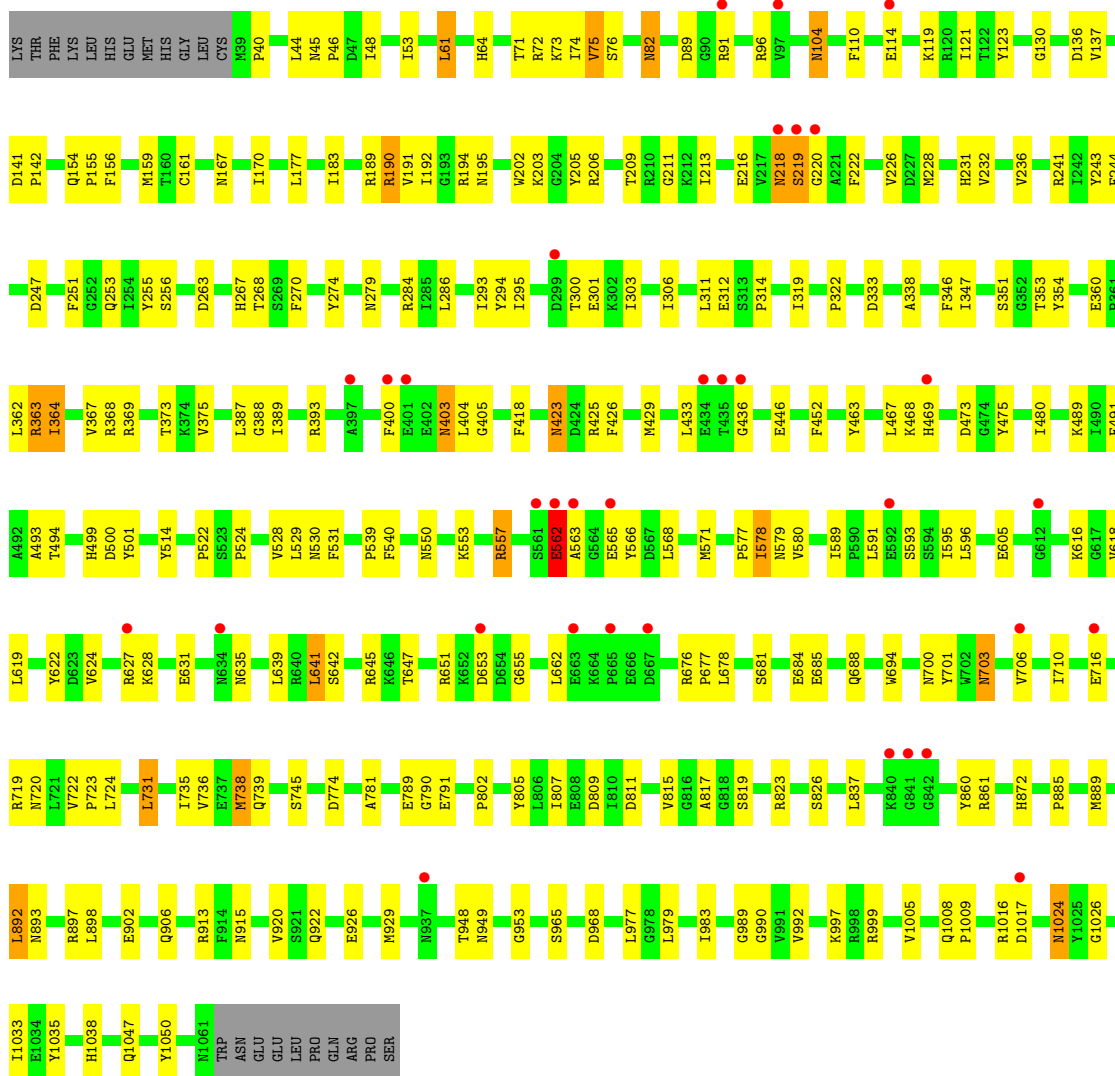
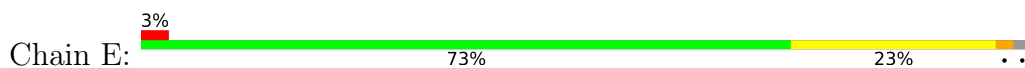


• Molecule 1: tricorn protease



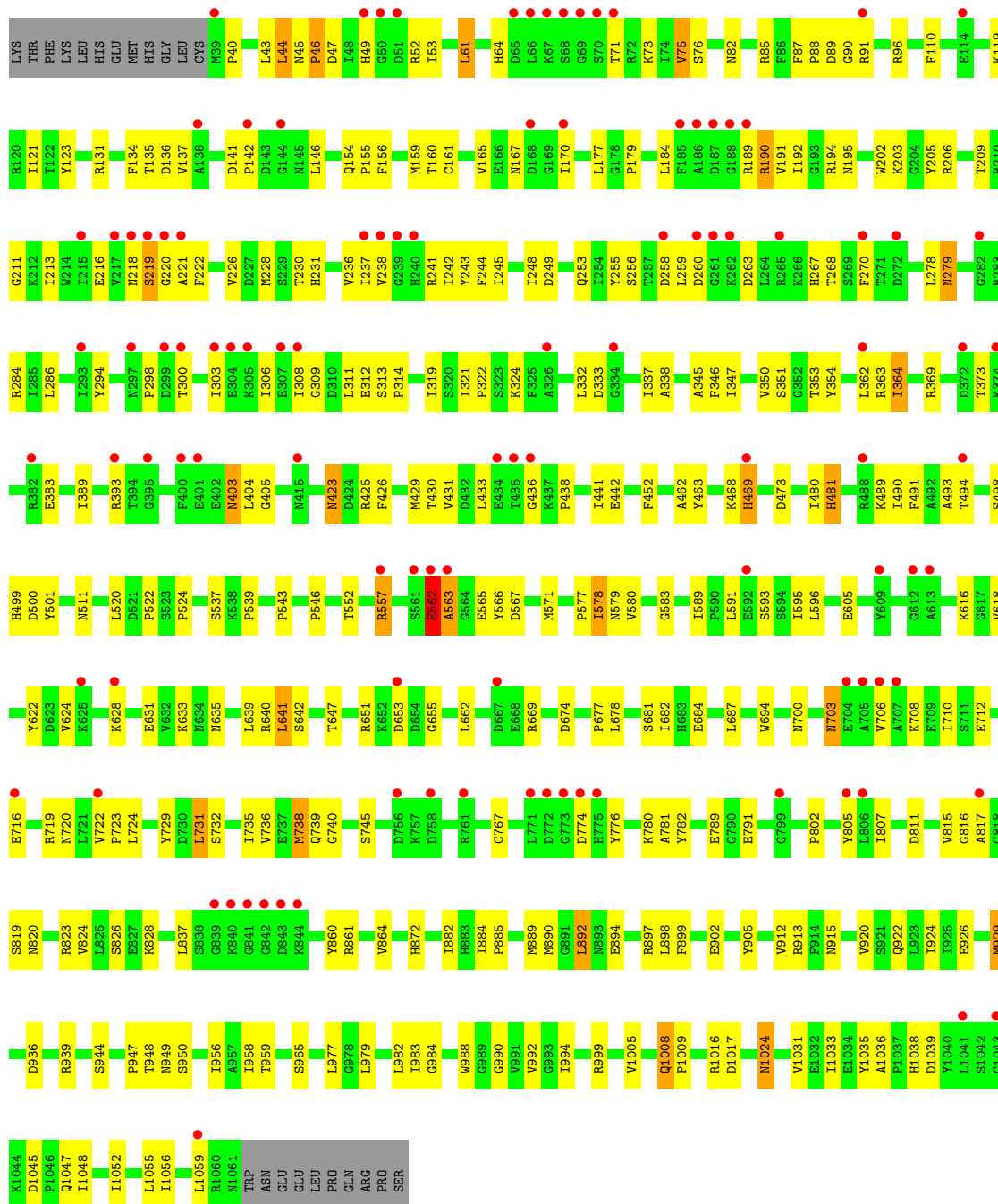


• Molecule 1: tricorn protease



• Molecule 1: tricorn protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.86Å 246.00Å 159.04Å 90.00° 105.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 37.48 – 1.98	Depositor EDS
% Data completeness (in resolution range)	78.6 (20.00-2.00) 81.6 (37.48-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.98Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.264 0.253 , 0.290	Depositor DCC
R_{free} test set	20086 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	51456	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/8367	0.66	1/11311 (0.0%)
1	B	0.40	0/8367	0.66	2/11311 (0.0%)
1	C	0.36	0/8367	0.62	1/11311 (0.0%)
1	D	0.39	0/8367	0.65	1/11311 (0.0%)
1	E	0.38	0/8367	0.65	1/11311 (0.0%)
1	F	0.36	0/8367	0.62	1/11311 (0.0%)
All	All	0.38	0/50202	0.64	7/67866 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	364	ILE	N-CA-C	-6.20	94.25	111.00
1	A	364	ILE	N-CA-C	-5.63	95.81	111.00
1	E	364	ILE	N-CA-C	-5.41	96.39	111.00
1	B	79	GLY	N-CA-C	-5.28	99.89	113.10
1	D	364	ILE	N-CA-C	-5.23	96.87	111.00
1	B	364	ILE	N-CA-C	-5.15	97.10	111.00
1	F	364	ILE	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8177	0	8003	256	0
1	B	8177	0	8003	265	0
1	C	8177	0	8003	272	0
1	D	8177	0	8003	226	0
1	E	8177	0	8003	249	0
1	F	8177	0	8003	275	0
2	A	401	0	0	12	0
2	B	395	0	0	8	0
2	C	398	0	0	18	0
2	D	401	0	0	9	0
2	E	405	0	0	10	0
2	F	394	0	0	10	0
All	All	51456	0	48018	1453	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 15.

All (1453) 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:F:155:PRO:HG2	1:F:159:MET:HE1	1.33	1.09
1:B:155:PRO:HG2	1:B:159:MET:HE1	1.36	1.07
1:C:155:PRO:HG2	1:C:159:MET:HE1	1.37	1.06
1:D:155:PRO:HG2	1:D:159:MET:HE1	1.35	1.03
1:B:983:ILE:HG23	1:B:1033:ILE:HD13	1.41	1.02
1:A:983:ILE:HG23	1:A:1033:ILE:HD13	1.41	0.99
1:D:983:ILE:HG23	1:D:1033:ILE:HD12	1.43	0.97
1:A:155:PRO:HG2	1:A:159:MET:HE1	1.46	0.95
1:F:154:GLN:HB3	1:F:159:MET:HE3	1.47	0.95
1:C:983:ILE:HG23	1:C:1033:ILE:HD13	1.49	0.94
1:B:104:ASN:HD22	1:B:104:ASN:H	1.12	0.93
1:D:53:ILE:HG23	1:D:286:LEU:HD21	1.48	0.93
1:A:948:THR:H	1:B:922:GLN:HE22	1.16	0.92
1:E:155:PRO:HG2	1:E:159:MET:HE1	1.49	0.91
1:F:983:ILE:HG23	1:F:1033:ILE:HD13	1.50	0.90
1:E:53:ILE:HG23	1:E:286:LEU:HD21	1.53	0.89
1:B:253:GLN:HE22	1:B:270:PHE:H	1.20	0.89
1:A:922:GLN:HE22	1:B:948:THR:H	1.21	0.88
1:C:154:GLN:HB3	1:C:159:MET:HE3	1.54	0.88
1:A:789:GLU:HG3	1:B:577:PRO:HG3	1.55	0.87
1:D:253:GLN:HE22	1:D:270:PHE:H	1.23	0.87
1:C:922:GLN:HE22	1:D:948:THR:H	1.15	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ILE:H	1:B:494:THR:HG22	1.38	0.87
1:B:468:LYS:HD2	1:B:473:ASP:HB2	1.58	0.86
1:F:480:ILE:H	1:F:494:THR:HG22	1.39	0.86
1:C:268:THR:HG22	1:C:303:ILE:HD11	1.56	0.85
1:E:104:ASN:HD22	1:E:104:ASN:H	1.23	0.85
1:F:468:LYS:HD2	1:F:473:ASP:HB2	1.57	0.85
1:B:539:PRO:HG2	1:B:578:ILE:HG23	1.58	0.85
1:C:104:ASN:HD22	1:C:104:ASN:H	1.22	0.85
1:E:922:GLN:HE22	1:F:948:THR:H	1.22	0.85
1:A:161:CYS:SG	2:A:2394:HOH:O	2.35	0.84
1:A:104:ASN:H	1:A:104:ASN:HD22	1.21	0.84
1:F:539:PRO:HG2	1:F:578:ILE:HG23	1.56	0.84
1:A:480:ILE:H	1:A:494:THR:HG22	1.41	0.84
1:C:73:LYS:HD3	1:C:76:SER:HB3	1.60	0.84
1:F:73:LYS:HD3	1:F:76:SER:HB3	1.59	0.83
1:F:322:PRO:HB3	1:F:678:LEU:HD13	1.59	0.83
1:E:40:PRO:HG2	1:E:724:LEU:HD22	1.59	0.83
1:E:403:ASN:ND2	1:E:405:GLY:H	1.76	0.83
1:D:104:ASN:H	1:D:104:ASN:HD22	1.26	0.82
1:A:253:GLN:HE22	1:A:270:PHE:H	1.22	0.81
1:E:983:ILE:HG23	1:E:1033:ILE:HD12	1.63	0.81
1:B:489:LYS:HG3	1:B:491:PHE:CE1	2.15	0.81
1:E:789:GLU:HG3	1:F:577:PRO:HG3	1.61	0.81
1:E:948:THR:H	1:F:922:GLN:HE22	1.29	0.81
1:C:40:PRO:HG2	1:C:724:LEU:HD22	1.61	0.80
1:F:268:THR:HG22	1:F:303:ILE:HD11	1.62	0.80
1:D:468:LYS:HD2	1:D:473:ASP:HB2	1.63	0.80
1:A:322:PRO:HG3	1:A:678:LEU:HD13	1.63	0.80
1:D:48:ILE:HB	1:D:286:LEU:HD22	1.64	0.79
1:F:404:LEU:HD22	1:F:429:MET:HE2	1.65	0.79
1:B:284:ARG:HD3	2:B:3393:HOH:O	1.81	0.78
1:C:577:PRO:HG3	1:D:789:GLU:HG3	1.63	0.78
1:E:539:PRO:HG2	1:E:578:ILE:HG23	1.65	0.78
1:A:557:ARG:NH2	1:E:393:ARG:HH12	1.80	0.78
1:B:161:CYS:SG	2:B:3394:HOH:O	2.40	0.78
1:E:154:GLN:HB3	1:E:159:MET:HE3	1.65	0.78
1:A:948:THR:H	1:B:922:GLN:NE2	1.82	0.78
1:A:404:LEU:HD22	1:A:429:MET:HE2	1.66	0.77
1:B:154:GLN:HB3	1:B:159:MET:HE3	1.67	0.77
1:F:403:ASN:ND2	1:F:405:GLY:H	1.82	0.77
1:D:662:LEU:O	1:D:662:LEU:HD23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:CYS:SG	2:E:6394:HOH:O	2.42	0.77
1:F:694:TRP:HA	1:F:738:MET:CE	2.15	0.77
1:C:403:ASN:HD22	1:C:405:GLY:H	1.33	0.77
1:C:403:ASN:ND2	1:C:405:GLY:H	1.81	0.77
1:F:253:GLN:HE22	1:F:270:PHE:H	1.33	0.77
1:A:268:THR:HG22	1:A:303:ILE:HD11	1.67	0.76
1:C:539:PRO:HG2	1:C:578:ILE:HG23	1.66	0.76
1:C:480:ILE:H	1:C:494:THR:HG22	1.50	0.76
1:A:73:LYS:HD3	1:A:76:SER:HB3	1.67	0.76
1:A:293:ILE:HG22	1:A:306:ILE:HD12	1.68	0.76
1:C:578:ILE:HG12	1:C:580:VAL:HG23	1.67	0.76
1:A:284:ARG:HD3	2:A:2393:HOH:O	1.84	0.76
1:E:662:LEU:HD23	1:E:662:LEU:O	1.86	0.76
1:B:73:LYS:HD3	1:B:76:SER:HB3	1.68	0.76
1:B:206:ARG:H	1:B:1024:ASN:HD21	1.32	0.75
1:D:40:PRO:HG2	1:D:724:LEU:HD22	1.67	0.75
1:A:539:PRO:HG2	1:A:578:ILE:HG23	1.68	0.75
1:F:403:ASN:HD22	1:F:405:GLY:H	1.35	0.75
1:F:350:VAL:HG21	1:F:669:ARG:HH11	1.51	0.75
1:C:948:THR:H	1:D:922:GLN:HE22	1.33	0.75
1:F:82:ASN:HD21	1:F:96:ARG:HH21	1.33	0.75
1:A:154:GLN:HB3	1:A:159:MET:HE3	1.69	0.74
1:D:53:ILE:CG2	1:D:286:LEU:HD21	2.16	0.74
1:E:403:ASN:HD22	1:E:405:GLY:H	1.35	0.74
1:C:167:ASN:HB2	1:C:170:ILE:HB	1.68	0.74
1:C:286:LEU:HD12	1:C:294:TYR:O	1.87	0.74
1:A:353:THR:HG23	1:A:354:TYR:CD1	2.23	0.74
1:A:489:LYS:HG3	1:A:491:PHE:CE1	2.22	0.74
1:E:253:GLN:HE22	1:E:270:PHE:H	1.34	0.74
1:B:206:ARG:H	1:B:1024:ASN:ND2	1.85	0.74
1:B:295:ILE:HG13	1:B:306:ILE:HD11	1.68	0.74
1:D:268:THR:HG22	1:D:303:ILE:HD11	1.69	0.74
1:B:480:ILE:H	1:B:494:THR:CG2	2.00	0.73
1:A:40:PRO:HG2	1:A:724:LEU:HD22	1.69	0.73
1:D:578:ILE:HG12	1:D:580:VAL:HG23	1.70	0.73
1:F:206:ARG:H	1:F:1024:ASN:ND2	1.86	0.73
1:E:268:THR:HG22	1:E:303:ILE:HD11	1.69	0.73
1:E:480:ILE:H	1:E:494:THR:HG22	1.54	0.73
1:A:468:LYS:HD2	1:A:473:ASP:HB2	1.70	0.73
1:B:286:LEU:HD12	1:B:294:TYR:O	1.88	0.73
1:F:206:ARG:H	1:F:1024:ASN:HD21	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:TRP:CH2	1:B:745:SER:HB3	2.24	0.72
1:C:468:LYS:HD2	1:C:473:ASP:HB2	1.70	0.72
1:F:578:ILE:HG12	1:F:580:VAL:HG23	1.70	0.72
1:B:350:VAL:HG21	1:B:669:ARG:HH11	1.53	0.72
1:B:351:SER:OG	1:B:353:THR:HG22	1.88	0.72
1:C:161:CYS:SG	2:C:4394:HOH:O	2.47	0.72
1:E:922:GLN:NE2	1:F:948:THR:H	1.86	0.72
1:A:350:VAL:HG21	1:A:669:ARG:HH11	1.54	0.72
1:B:681:SER:HB3	1:B:684:GLU:HG2	1.70	0.72
1:B:40:PRO:HG2	1:B:724:LEU:HD22	1.72	0.71
1:D:161:CYS:SG	2:D:5394:HOH:O	2.48	0.71
1:F:155:PRO:CG	1:F:159:MET:HE1	2.17	0.71
1:F:286:LEU:HD12	1:F:294:TYR:O	1.90	0.71
1:C:253:GLN:HE22	1:C:270:PHE:H	1.37	0.71
1:A:351:SER:OG	1:A:353:THR:HG22	1.91	0.71
1:C:694:TRP:HA	1:C:738:MET:CE	2.21	0.71
1:D:73:LYS:HD3	1:D:76:SER:HB3	1.73	0.71
1:D:403:ASN:ND2	1:D:405:GLY:H	1.87	0.71
1:A:480:ILE:H	1:A:494:THR:CG2	2.04	0.71
1:A:206:ARG:H	1:A:1024:ASN:ND2	1.88	0.71
1:A:922:GLN:NE2	1:B:948:THR:H	1.86	0.71
1:D:404:LEU:HD22	1:D:429:MET:HE2	1.72	0.70
1:D:403:ASN:HD22	1:D:405:GLY:H	1.38	0.70
1:A:205:TYR:HA	1:A:1024:ASN:HD21	1.57	0.70
1:C:322:PRO:HB3	1:C:678:LEU:HD13	1.72	0.69
1:E:468:LYS:HD2	1:E:473:ASP:HB2	1.74	0.69
1:B:268:THR:HG22	1:B:303:ILE:HD11	1.71	0.69
1:F:82:ASN:ND2	1:F:96:ARG:HH21	1.90	0.69
1:B:82:ASN:ND2	1:B:96:ARG:HH21	1.90	0.69
1:F:40:PRO:HG2	1:F:724:LEU:CD2	2.21	0.69
1:D:206:ARG:H	1:D:1024:ASN:ND2	1.90	0.69
1:F:662:LEU:HD23	1:F:662:LEU:O	1.92	0.69
1:B:557:ARG:NE	1:D:393:ARG:HH22	1.91	0.69
1:D:351:SER:OG	1:D:353:THR:HG22	1.93	0.69
1:F:61:LEU:HB3	1:F:75:VAL:HG13	1.73	0.69
1:A:577:PRO:HG3	1:B:789:GLU:HG3	1.75	0.68
1:F:774:ASP:HA	1:F:817:ALA:HB2	1.74	0.68
1:D:404:LEU:HD22	1:D:429:MET:CE	2.22	0.68
1:A:393:ARG:HH22	1:C:557:ARG:NE	1.91	0.68
1:B:430:THR:HG23	1:B:441:ILE:HD11	1.75	0.68
1:B:404:LEU:HD22	1:B:429:MET:HE2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:ASN:ND2	1:E:531:PHE:H	1.90	0.68
1:C:350:VAL:HG21	1:C:669:ARG:HH11	1.58	0.68
1:B:363:ARG:HG3	1:B:688:GLN:NE2	2.09	0.68
1:F:480:ILE:H	1:F:494:THR:CG2	2.07	0.68
1:F:892:LEU:HD13	1:F:920:VAL:HG21	1.73	0.68
1:C:681:SER:HB3	1:C:684:GLU:HG2	1.74	0.68
1:A:53:ILE:HG23	1:A:286:LEU:HD21	1.75	0.68
1:D:977:LEU:HB2	1:D:979:LEU:CD1	2.24	0.68
1:E:73:LYS:HD3	1:E:76:SER:HB3	1.74	0.68
1:D:190:ARG:NH2	1:D:222:PHE:HZ	1.93	0.67
1:E:322:PRO:HG3	1:E:678:LEU:HD13	1.75	0.67
1:E:53:ILE:CG2	1:E:286:LEU:HD21	2.23	0.67
1:E:205:TYR:HA	1:E:1024:ASN:HD21	1.58	0.67
1:F:351:SER:OG	1:F:353:THR:HG22	1.93	0.67
1:B:40:PRO:HG2	1:B:724:LEU:CD2	2.24	0.67
1:C:635:ASN:HB3	1:C:653:ASP:OD1	1.95	0.67
1:C:922:GLN:NE2	1:D:948:THR:H	1.89	0.67
1:F:236:VAL:HG23	1:F:243:TYR:HB2	1.76	0.67
1:A:222:PHE:H	1:A:1038:HIS:HD2	1.42	0.67
1:C:190:ARG:NH2	1:C:222:PHE:HZ	1.91	0.67
1:B:404:LEU:HD22	1:B:429:MET:CE	2.24	0.67
1:D:703:ASN:C	1:D:703:ASN:HD22	1.98	0.67
1:A:350:VAL:HG21	1:A:669:ARG:NH1	2.10	0.67
1:E:190:ARG:NH2	1:E:222:PHE:HZ	1.93	0.67
1:B:72:ARG:HG3	1:E:72:ARG:HG3	1.75	0.67
1:F:53:ILE:HG23	1:F:286:LEU:HD21	1.77	0.67
1:F:982:LEU:O	1:F:983:ILE:HD12	1.95	0.66
1:A:393:ARG:HH12	1:C:557:ARG:HD2	1.59	0.66
1:D:913:ARG:HH21	1:D:1047:GLN:HE21	1.42	0.66
1:D:480:ILE:H	1:D:494:THR:HG22	1.60	0.66
1:D:681:SER:O	1:D:684:GLU:HG2	1.95	0.66
1:B:489:LYS:HG3	1:B:491:PHE:HE1	1.57	0.66
1:D:154:GLN:HB3	1:D:159:MET:HE3	1.78	0.66
1:D:286:LEU:HD12	1:D:294:TYR:O	1.96	0.66
1:A:681:SER:HB3	1:A:684:GLU:HG2	1.77	0.66
1:D:539:PRO:HG2	1:D:578:ILE:HG23	1.76	0.66
1:D:40:PRO:HG2	1:D:724:LEU:CD2	2.26	0.66
1:D:206:ARG:H	1:D:1024:ASN:HD21	1.43	0.66
1:E:284:ARG:HD3	2:E:6393:HOH:O	1.95	0.66
1:F:977:LEU:HB2	1:F:979:LEU:HD13	1.78	0.66
1:A:893:ASN:OD1	1:B:522:PRO:HD3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:403:ASN:HD22	1:E:403:ASN:C	1.99	0.66
1:A:522:PRO:HD3	1:B:893:ASN:OD1	1.95	0.65
1:E:404:LEU:HD22	1:E:429:MET:HE2	1.77	0.65
1:C:61:LEU:CB	1:C:75:VAL:HG13	2.26	0.65
1:D:61:LEU:CB	1:D:75:VAL:HG13	2.26	0.65
1:E:48:ILE:HB	1:E:286:LEU:HD22	1.77	0.65
1:F:628:LYS:HE3	2:F:7366:HOH:O	1.95	0.65
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.26	0.65
1:D:446:GLU:OE1	1:D:468:LYS:HE2	1.97	0.65
1:E:206:ARG:H	1:E:1024:ASN:ND2	1.94	0.65
1:B:256:SER:OG	1:B:267:HIS:HE1	1.80	0.65
1:B:593:SER:O	1:B:624:VAL:HG22	1.96	0.65
1:B:774:ASP:HA	1:B:817:ALA:HB2	1.78	0.65
1:F:982:LEU:C	1:F:983:ILE:HD12	2.17	0.65
1:B:53:ILE:HG23	1:B:286:LEU:HD21	1.79	0.64
1:E:591:LEU:HD11	1:E:662:LEU:HD21	1.79	0.64
1:F:179:PRO:HG2	2:F:7045:HOH:O	1.96	0.64
1:A:552:THR:HG21	1:A:578:ILE:HD12	1.78	0.64
1:B:61:LEU:CB	1:B:75:VAL:HG13	2.27	0.64
1:C:74:ILE:HG13	1:C:75:VAL:HG12	1.78	0.64
1:C:480:ILE:H	1:C:494:THR:CG2	2.10	0.64
1:C:662:LEU:HD23	1:C:662:LEU:O	1.96	0.64
1:E:293:ILE:HG22	1:E:306:ILE:HD12	1.78	0.64
1:B:82:ASN:HD21	1:B:96:ARG:HH21	1.45	0.64
1:E:353:THR:HG23	1:E:354:TYR:CD1	2.32	0.64
1:F:161:CYS:SG	2:F:7394:HOH:O	2.55	0.64
1:F:694:TRP:HA	1:F:738:MET:HE1	1.78	0.64
1:C:322:PRO:HA	1:C:678:LEU:HD22	1.80	0.64
1:D:530:ASN:ND2	1:D:531:PHE:H	1.96	0.64
1:A:46:PRO:HB2	1:A:286:LEU:HD21	1.80	0.64
1:A:286:LEU:HD12	1:A:294:TYR:O	1.97	0.64
1:B:46:PRO:HB2	1:B:286:LEU:CD2	2.27	0.64
1:A:628:LYS:HE3	2:A:2366:HOH:O	1.98	0.64
1:B:222:PHE:H	1:B:1038:HIS:HD2	1.46	0.64
1:A:46:PRO:HB2	1:A:286:LEU:CD2	2.28	0.64
1:A:774:ASP:HA	1:A:817:ALA:HB2	1.78	0.64
1:B:350:VAL:HG21	1:B:669:ARG:NH1	2.12	0.64
1:B:403:ASN:HD22	1:B:405:GLY:H	1.46	0.64
1:F:872:HIS:HE1	1:F:902:GLU:OE1	1.81	0.64
1:B:403:ASN:ND2	1:B:405:GLY:H	1.96	0.63
1:C:948:THR:H	1:D:922:GLN:NE2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:H	1:A:1024:ASN:HD21	1.44	0.63
1:C:104:ASN:H	1:C:104:ASN:ND2	1.94	0.63
1:C:694:TRP:HA	1:C:738:MET:HE1	1.79	0.63
1:A:493:ALA:HA	1:A:571:MET:HG3	1.79	0.63
1:A:815:VAL:HA	1:A:819:SER:HB3	1.81	0.63
1:C:40:PRO:HG2	1:C:724:LEU:CD2	2.28	0.63
1:C:155:PRO:CG	1:C:159:MET:HE1	2.21	0.63
1:A:789:GLU:OE2	2:A:2230:HOH:O	2.15	0.63
1:D:53:ILE:HG23	1:D:286:LEU:CD2	2.27	0.63
1:D:977:LEU:HB2	1:D:979:LEU:HD13	1.80	0.63
1:F:350:VAL:HG21	1:F:669:ARG:NH1	2.12	0.63
1:A:684:GLU:HG3	1:A:685:GLU:N	2.14	0.63
1:B:618:VAL:HG23	1:B:633:LYS:O	1.99	0.63
1:F:681:SER:O	1:F:684:GLU:HG2	1.99	0.63
1:B:353:THR:HG23	1:B:354:TYR:CD1	2.34	0.63
1:D:403:ASN:HD22	1:D:403:ASN:C	2.01	0.63
1:A:889:MET:SD	1:B:522:PRO:HG2	2.38	0.63
1:E:312:GLU:HG2	1:E:314:PRO:HD3	1.80	0.63
1:A:61:LEU:HB2	1:A:75:VAL:HG13	1.81	0.62
1:A:522:PRO:HG2	1:B:889:MET:SD	2.39	0.62
1:B:578:ILE:HG12	1:B:580:VAL:HG23	1.81	0.62
1:F:195:ASN:O	1:F:231:HIS:HE1	1.83	0.62
1:D:155:PRO:HG2	1:D:159:MET:CE	2.22	0.62
1:D:494:THR:HG21	1:D:500:ASP:OD1	1.99	0.62
1:F:40:PRO:HG2	1:F:724:LEU:HD22	1.82	0.62
1:A:40:PRO:HG2	1:A:724:LEU:CD2	2.29	0.62
1:B:241:ARG:NH1	1:B:263:ASP:OD1	2.33	0.62
1:B:319:ILE:HG23	1:B:677:PRO:HB3	1.80	0.62
1:C:403:ASN:HD22	1:C:403:ASN:C	2.03	0.62
1:F:61:LEU:CB	1:F:75:VAL:HG13	2.30	0.62
1:B:64:HIS:HD2	1:B:71:THR:OG1	1.82	0.62
1:C:628:LYS:HE3	2:C:4366:HOH:O	1.99	0.62
1:F:404:LEU:HD22	1:F:429:MET:CE	2.28	0.62
1:B:363:ARG:HD2	1:B:365:ARG:NH2	2.15	0.62
1:D:716:GLU:HG2	1:D:720:ASN:HD21	1.64	0.62
1:D:815:VAL:HA	1:D:819:SER:HB3	1.82	0.62
1:E:446:GLU:OE1	1:E:468:LYS:HE2	2.00	0.62
1:E:489:LYS:HG3	1:E:491:PHE:CE1	2.35	0.62
1:F:716:GLU:HG2	1:F:720:ASN:HD21	1.64	0.62
1:D:82:ASN:HD21	1:D:96:ARG:HH21	1.48	0.62
1:E:53:ILE:HD11	1:E:295:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:999:ARG:HG2	1:F:1005:VAL:HG22	1.81	0.62
1:A:489:LYS:HG3	1:A:491:PHE:HE1	1.65	0.61
1:A:189:ARG:HD2	1:A:216:GLU:O	1.99	0.61
1:B:913:ARG:HH21	1:B:1047:GLN:HE21	1.47	0.61
1:F:736:VAL:HA	1:F:739:GLN:HE21	1.64	0.61
1:A:387:LEU:HD13	1:A:388:GLY:N	2.15	0.61
1:E:130:GLY:HA3	2:E:6163:HOH:O	2.00	0.61
1:F:489:LYS:HG3	1:F:491:PHE:CE1	2.36	0.61
1:B:480:ILE:N	1:B:494:THR:HG22	2.12	0.61
1:C:256:SER:OG	1:C:267:HIS:HE1	1.84	0.61
1:E:716:GLU:HG2	1:E:720:ASN:ND2	2.16	0.61
1:A:403:ASN:ND2	1:A:405:GLY:H	1.97	0.61
1:D:489:LYS:HG3	1:D:491:PHE:CE1	2.35	0.61
1:D:694:TRP:HA	1:D:738:MET:CE	2.31	0.61
1:D:716:GLU:HG2	1:D:720:ASN:ND2	2.14	0.61
1:F:46:PRO:HB2	1:F:286:LEU:CD2	2.30	0.61
1:F:423:ASN:HD22	1:F:423:ASN:C	2.04	0.61
1:B:190:ARG:NH2	1:B:222:PHE:HZ	1.98	0.61
1:B:393:ARG:HH12	1:F:557:ARG:HD2	1.66	0.61
1:A:1031:VAL:HG12	1:A:1033:ILE:HD11	1.83	0.61
1:F:167:ASN:HB2	1:F:170:ILE:HB	1.83	0.61
1:A:241:ARG:NH1	1:A:263:ASP:OD1	2.33	0.61
1:F:253:GLN:HB2	1:F:255:TYR:CE1	2.36	0.61
1:C:236:VAL:HG23	1:C:243:TYR:HB2	1.82	0.60
1:E:53:ILE:HG23	1:E:286:LEU:CD2	2.29	0.60
1:E:635:ASN:HB3	1:E:653:ASP:OD1	2.01	0.60
1:B:393:ARG:HH12	1:F:557:ARG:CZ	2.13	0.60
1:E:404:LEU:HD22	1:E:429:MET:CE	2.31	0.60
1:A:662:LEU:HD23	1:A:662:LEU:O	2.02	0.60
1:C:279:ASN:ND2	2:C:4071:HOH:O	2.32	0.60
1:D:190:ARG:HH21	1:D:190:ARG:HB2	1.66	0.60
1:C:593:SER:O	1:C:624:VAL:HG22	2.00	0.60
1:D:61:LEU:HB2	1:D:75:VAL:HG13	1.82	0.60
1:F:694:TRP:HA	1:F:738:MET:HE2	1.84	0.60
1:E:40:PRO:HG2	1:E:724:LEU:CD2	2.32	0.60
1:A:498:SER:HB2	2:A:3192:HOH:O	2.01	0.60
1:B:155:PRO:CG	1:B:159:MET:HE1	2.22	0.60
1:E:977:LEU:HB2	1:E:979:LEU:HD13	1.84	0.60
1:B:684:GLU:HG3	1:B:685:GLU:N	2.16	0.60
1:C:195:ASN:O	1:C:231:HIS:HE1	1.85	0.60
1:C:681:SER:O	1:C:684:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:OG	1:A:267:HIS:HE1	1.84	0.60
1:C:423:ASN:C	1:C:423:ASN:HD22	2.04	0.60
1:B:322:PRO:HB3	1:B:678:LEU:HD13	1.83	0.59
1:E:206:ARG:H	1:E:1024:ASN:HD21	1.50	0.59
1:E:622:TYR:OH	1:E:627:ARG:HG2	2.01	0.59
1:A:230:THR:HG21	1:A:248:ILE:HA	1.84	0.59
1:A:480:ILE:N	1:A:494:THR:HG22	2.14	0.59
1:B:206:ARG:N	1:B:1024:ASN:HD21	2.00	0.59
1:C:872:HIS:HE1	1:C:902:GLU:OE1	1.85	0.59
1:E:716:GLU:HG2	1:E:720:ASN:HD21	1.66	0.59
1:C:309:GLY:O	1:C:311:LEU:HD13	2.03	0.59
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.32	0.59
1:A:222:PHE:H	1:A:1038:HIS:CD2	2.19	0.59
1:A:489:LYS:HE2	1:A:491:PHE:HZ	1.67	0.59
1:B:61:LEU:HB2	1:B:75:VAL:HG13	1.83	0.59
1:D:82:ASN:ND2	1:D:96:ARG:HH21	2.00	0.59
1:E:489:LYS:HE2	1:E:491:PHE:HZ	1.66	0.59
1:A:393:ARG:HH12	1:C:557:ARG:NH2	2.01	0.59
1:B:872:HIS:HE1	1:B:902:GLU:OE1	1.85	0.59
1:C:61:LEU:HB3	1:C:75:VAL:HG13	1.83	0.59
1:D:642:SER:HB2	1:D:647:THR:HB	1.83	0.59
1:B:662:LEU:O	1:B:662:LEU:HD23	2.02	0.59
1:E:155:PRO:HD2	1:E:159:MET:HE3	1.85	0.59
1:F:988:TRP:CZ3	1:F:990:GLY:HA3	2.38	0.59
1:A:202:TRP:CH2	1:A:745:SER:HB3	2.38	0.59
1:C:322:PRO:HG2	1:C:674:ASP:OD1	2.02	0.59
1:E:676:ARG:HD2	2:E:6370:HOH:O	2.02	0.59
1:B:46:PRO:HB2	1:B:286:LEU:HD21	1.85	0.59
1:C:404:LEU:HD22	1:C:429:MET:HE2	1.85	0.59
1:E:913:ARG:HH21	1:E:1047:GLN:HE21	1.49	0.59
1:F:256:SER:OG	1:F:267:HIS:HE1	1.86	0.59
1:F:1045:ASP:HB3	1:F:1048:ILE:HG22	1.85	0.59
1:A:64:HIS:HD2	1:A:71:THR:OG1	1.85	0.59
1:C:999:ARG:HG2	1:C:1005:VAL:HG22	1.84	0.59
1:F:52:ARG:HH21	1:F:52:ARG:HG3	1.68	0.59
1:E:61:LEU:CB	1:E:75:VAL:HG13	2.33	0.58
1:E:82:ASN:HD21	1:E:96:ARG:HH21	1.51	0.58
1:B:589:ILE:HD13	1:B:641:LEU:HD12	1.85	0.58
1:E:681:SER:O	1:E:684:GLU:HG2	2.03	0.58
1:D:190:ARG:NH2	1:D:222:PHE:CZ	2.71	0.58
1:D:190:ARG:NH2	1:D:216:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:SER:OG	1:D:267:HIS:HE1	1.86	0.58
1:E:681:SER:HB3	1:E:684:GLU:HG2	1.85	0.58
1:D:622:TYR:OH	1:D:627:ARG:HG2	2.03	0.58
1:E:82:ASN:ND2	1:E:96:ARG:HH21	2.01	0.58
1:A:82:ASN:ND2	1:A:96:ARG:HH21	2.01	0.58
1:B:119:LYS:NZ	1:B:823:ARG:HH22	2.01	0.58
1:B:628:LYS:HE3	2:B:3366:HOH:O	2.03	0.58
1:E:333:ASP:CG	1:E:369:ARG:HE	2.06	0.58
1:B:293:ILE:HG22	1:B:306:ILE:HD12	1.86	0.58
1:C:889:MET:SD	1:D:522:PRO:HG2	2.44	0.58
1:C:947:PRO:HD2	1:C:950:SER:HB3	1.86	0.58
1:E:61:LEU:HB3	1:E:75:VAL:HG13	1.84	0.58
1:C:43:LEU:O	1:C:44:LEU:HG	2.04	0.58
1:D:872:HIS:HE1	1:D:902:GLU:OE1	1.86	0.58
1:F:403:ASN:HD22	1:F:403:ASN:C	2.07	0.58
1:B:781:ALA:HB2	1:B:802:PRO:HG2	1.86	0.58
1:E:190:ARG:NH2	1:E:222:PHE:CZ	2.72	0.58
1:B:104:ASN:H	1:B:104:ASN:ND2	1.89	0.57
1:E:64:HIS:HD2	1:E:71:THR:OG1	1.87	0.57
1:F:319:ILE:HG23	1:F:677:PRO:HB3	1.85	0.57
1:F:815:VAL:HA	1:F:819:SER:HB3	1.85	0.57
1:A:872:HIS:HE1	1:A:902:GLU:OE1	1.87	0.57
1:C:530:ASN:ND2	1:C:531:PHE:H	2.02	0.57
1:D:322:PRO:HB3	1:D:678:LEU:HD13	1.85	0.57
1:E:104:ASN:HD22	1:E:104:ASN:N	1.91	0.57
1:E:104:ASN:H	1:E:104:ASN:ND2	1.99	0.57
1:E:694:TRP:HA	1:E:738:MET:CE	2.34	0.57
1:F:884:ILE:HD13	1:F:924:ILE:HD13	1.86	0.57
1:D:635:ASN:HB3	1:D:653:ASP:OD1	2.04	0.57
1:F:618:VAL:HG23	1:F:633:LYS:O	2.03	0.57
1:F:735:ILE:O	1:F:739:GLN:HG3	2.04	0.57
1:E:202:TRP:CH2	1:E:745:SER:HB3	2.39	0.57
1:F:218:ASN:O	1:F:219:SER:C	2.43	0.57
1:F:947:PRO:HD2	1:F:950:SER:HB3	1.85	0.57
1:A:319:ILE:HG23	1:A:677:PRO:HB3	1.87	0.57
1:B:390:TYR:HD1	1:B:397:ALA:HB2	1.69	0.57
1:B:557:ARG:CZ	1:D:393:ARG:HH12	2.18	0.57
1:C:524:PRO:HD3	1:D:605:GLU:HG2	1.87	0.57
1:D:965:SER:HA	1:D:990:GLY:O	2.03	0.57
1:F:350:VAL:CG2	1:F:669:ARG:HH11	2.15	0.57
1:E:815:VAL:HA	1:E:819:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:THR:HG21	1:C:248:ILE:HA	1.87	0.57
1:D:684:GLU:HG3	1:D:685:GLU:N	2.19	0.57
1:A:346:PHE:C	1:A:347:ILE:HD12	2.25	0.56
1:C:319:ILE:HG23	1:C:677:PRO:HB3	1.86	0.56
1:D:241:ARG:NH1	1:D:263:ASP:OD1	2.37	0.56
1:D:489:LYS:HG3	1:D:491:PHE:HE1	1.70	0.56
1:F:642:SER:HB2	1:F:647:THR:HB	1.87	0.56
1:C:350:VAL:HG21	1:C:669:ARG:NH1	2.19	0.56
1:D:360:GLU:HB2	1:D:364:ILE:HD11	1.86	0.56
1:D:694:TRP:HA	1:D:738:MET:HE1	1.87	0.56
1:E:232:VAL:HG13	1:E:244:PHE:CD1	2.41	0.56
1:E:351:SER:OG	1:E:353:THR:HG22	2.05	0.56
1:E:807:ILE:HG12	1:E:837:LEU:CD2	2.35	0.56
1:F:216:GLU:OE1	1:F:219:SER:HA	2.05	0.56
1:F:202:TRP:CH2	1:F:745:SER:HB3	2.40	0.56
1:F:308:ILE:HG22	1:F:311:LEU:HD11	1.87	0.56
1:A:104:ASN:H	1:A:104:ASN:ND2	1.98	0.56
1:B:489:LYS:HE2	1:B:491:PHE:HZ	1.71	0.56
1:B:811:ASP:OD1	1:E:676:ARG:NH1	2.39	0.56
1:D:205:TYR:HA	1:D:1024:ASN:HD21	1.70	0.56
1:F:562:GLU:O	1:F:563:ALA:HB3	2.06	0.56
1:A:605:GLU:CG	1:B:524:PRO:HD3	2.36	0.56
1:B:153:MET:HG3	1:B:859:ARG:CZ	2.35	0.56
1:F:312:GLU:HG2	1:F:314:PRO:HD3	1.87	0.56
1:D:999:ARG:HG2	1:D:1005:VAL:HG22	1.86	0.56
1:F:965:SER:HA	1:F:990:GLY:O	2.06	0.56
1:A:423:ASN:C	1:A:423:ASN:HD22	2.09	0.56
1:D:284:ARG:HD3	2:D:5393:HOH:O	2.05	0.56
1:F:353:THR:HG23	1:F:354:TYR:CD1	2.40	0.56
1:A:429:MET:HE3	1:A:438:PRO:HB2	1.87	0.56
1:A:965:SER:HA	1:A:990:GLY:O	2.06	0.56
1:B:499:HIS:HD2	2:B:3176:HOH:O	1.89	0.56
1:D:312:GLU:HG2	1:D:314:PRO:HD3	1.86	0.56
1:E:568:LEU:HB3	1:E:571:MET:HE2	1.87	0.56
1:E:872:HIS:HE1	1:E:902:GLU:OE1	1.89	0.56
1:E:1016:ARG:O	1:E:1017:ASP:HB2	2.06	0.56
1:A:403:ASN:HD22	1:A:405:GLY:H	1.54	0.55
1:E:499:HIS:HE1	2:E:6239:HOH:O	1.89	0.55
1:B:493:ALA:HA	1:B:571:MET:HG3	1.88	0.55
1:B:977:LEU:HB2	1:B:979:LEU:HD13	1.88	0.55
1:C:53:ILE:HG23	1:C:286:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:929:MET:CE	1:C:929:MET:HA	2.36	0.55
1:D:353:THR:HG23	1:D:354:TYR:CD1	2.41	0.55
1:E:605:GLU:HG2	1:F:524:PRO:HD3	1.88	0.55
1:A:293:ILE:CG2	1:A:306:ILE:HD12	2.36	0.55
1:B:167:ASN:HB2	1:B:170:ILE:HB	1.87	0.55
1:C:565:GLU:HG2	1:C:566:TYR:N	2.21	0.55
1:E:190:ARG:NH2	1:E:216:GLU:OE2	2.40	0.55
1:E:593:SER:O	1:E:624:VAL:HG22	2.05	0.55
1:A:681:SER:O	1:A:684:GLU:HG2	2.06	0.55
1:B:494:THR:HG21	1:B:500:ASP:OD1	2.06	0.55
1:F:635:ASN:HB3	1:F:653:ASP:OD1	2.07	0.55
1:D:929:MET:HA	1:D:929:MET:CE	2.36	0.55
1:D:184:LEU:HB2	1:D:191:VAL:HB	1.88	0.55
1:E:731:LEU:HD22	1:E:735:ILE:HG13	1.88	0.55
1:F:236:VAL:CG2	1:F:243:TYR:HB2	2.36	0.55
1:F:431:VAL:HG22	1:F:438:PRO:HB3	1.88	0.55
1:B:228:MET:HE3	1:B:232:VAL:CG2	2.36	0.55
1:B:423:ASN:C	1:B:423:ASN:HD22	2.09	0.55
1:C:522:PRO:HD3	1:D:893:ASN:OD1	2.05	0.55
1:E:480:ILE:H	1:E:494:THR:CG2	2.18	0.55
1:F:565:GLU:HG2	1:F:566:TYR:N	2.21	0.55
1:D:346:PHE:C	1:D:347:ILE:HD12	2.27	0.55
1:E:494:THR:HG21	1:E:500:ASP:OD1	2.07	0.55
1:F:258:ASP:C	1:F:260:ASP:H	2.10	0.55
1:A:155:PRO:HD2	1:A:159:MET:HE3	1.88	0.55
1:B:189:ARG:HD2	1:B:216:GLU:O	2.07	0.55
1:E:286:LEU:CD1	1:E:295:ILE:HG12	2.36	0.55
1:F:913:ARG:HH21	1:F:1047:GLN:HE21	1.55	0.55
1:B:88:PRO:HG3	1:B:144:GLY:HA2	1.89	0.55
1:B:155:PRO:HG2	1:B:159:MET:CE	2.25	0.55
1:A:119:LYS:NZ	1:A:823:ARG:HH22	2.05	0.54
1:B:892:LEU:HD13	1:B:920:VAL:HG21	1.89	0.54
1:C:694:TRP:HA	1:C:738:MET:HE2	1.87	0.54
1:D:295:ILE:HG13	1:D:306:ILE:HD11	1.87	0.54
1:C:965:SER:HA	1:C:990:GLY:O	2.08	0.54
1:D:565:GLU:HG2	1:D:566:TYR:N	2.22	0.54
1:C:321:ILE:HB	1:C:324:LYS:HG3	1.89	0.54
1:D:681:SER:HB3	1:D:684:GLU:HG2	1.88	0.54
1:F:43:LEU:O	1:F:44:LEU:HG	2.08	0.54
1:F:618:VAL:HG21	1:F:631:GLU:HG3	1.89	0.54
1:C:61:LEU:HB2	1:C:75:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ARG:HB2	1:C:243:TYR:CE1	2.42	0.54
1:C:774:ASP:HA	1:C:817:ALA:HB2	1.88	0.54
1:F:489:LYS:HG3	1:F:491:PHE:HE1	1.71	0.54
1:F:872:HIS:CE1	1:F:902:GLU:OE1	2.61	0.54
1:A:220:GLY:O	1:A:1038:HIS:HB3	2.08	0.54
1:E:155:PRO:CD	1:E:159:MET:HE3	2.38	0.54
1:E:530:ASN:ND2	1:E:531:PHE:N	2.55	0.54
1:D:591:LEU:HD11	1:D:662:LEU:HD21	1.89	0.54
1:E:167:ASN:HB2	1:E:170:ILE:HB	1.90	0.54
1:A:524:PRO:HD3	1:B:605:GLU:CG	2.36	0.54
1:A:736:VAL:HA	1:A:739:GLN:HE21	1.72	0.54
1:D:104:ASN:H	1:D:104:ASN:ND2	2.00	0.54
1:D:480:ILE:H	1:D:494:THR:CG2	2.19	0.54
1:E:948:THR:H	1:F:922:GLN:NE2	2.03	0.54
1:F:332:LEU:HD11	1:F:338:ALA:HB2	1.90	0.54
1:A:706:VAL:HG12	1:A:710:ILE:HD12	1.89	0.54
1:B:676:ARG:NH1	1:E:811:ASP:OD1	2.41	0.54
1:C:351:SER:OG	1:C:353:THR:HG22	2.07	0.54
1:C:589:ILE:HG21	1:C:641:LEU:HD11	1.89	0.54
1:C:700:ASN:HD22	1:C:1008:GLN:NE2	2.06	0.54
1:D:983:ILE:CG2	1:D:1033:ILE:HD12	2.28	0.54
1:E:156:PHE:CD1	1:E:159:MET:HE1	2.43	0.54
1:F:49:HIS:CD2	1:F:90:GLY:HA3	2.43	0.54
1:F:184:LEU:HD13	1:F:237:ILE:HG13	1.90	0.54
1:F:498:SER:OG	1:F:499:HIS:N	2.40	0.54
1:B:546:PRO:CG	1:B:567:ASP:HB3	2.38	0.54
1:C:562:GLU:O	1:C:563:ALA:HB3	2.08	0.54
1:B:703:ASN:HD22	1:B:703:ASN:C	2.12	0.54
1:C:206:ARG:H	1:C:1024:ASN:ND2	2.06	0.54
1:D:64:HIS:HD2	1:D:71:THR:OG1	1.91	0.54
1:D:807:ILE:HG12	1:D:837:LEU:CD2	2.38	0.54
1:F:1036:ALA:O	1:F:1039:ASP:HB2	2.08	0.54
1:E:286:LEU:HD12	1:E:294:TYR:O	2.07	0.53
1:F:87:PHE:HB3	1:F:88:PRO:HD2	1.90	0.53
1:A:494:THR:HG21	1:A:500:ASP:OD1	2.08	0.53
1:B:393:ARG:HH22	1:F:557:ARG:NE	2.06	0.53
1:F:222:PHE:H	1:F:1038:HIS:HD2	1.53	0.53
1:A:363:ARG:HG3	1:A:688:GLN:NE2	2.23	0.53
1:B:218:ASN:HB3	1:B:221:ALA:HB3	1.90	0.53
1:B:355:VAL:HG12	1:B:676:ARG:HH21	1.74	0.53
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:SER:CB	1:B:684:GLU:HG2	2.37	0.53
1:C:522:PRO:HG2	1:D:889:MET:SD	2.47	0.53
1:F:253:GLN:NE2	1:F:268:THR:OG1	2.39	0.53
1:A:703:ASN:C	1:A:703:ASN:HD22	2.11	0.53
1:B:789:GLU:OE2	2:B:3230:HOH:O	2.19	0.53
1:E:241:ARG:NH1	1:E:263:ASP:OD1	2.41	0.53
1:E:475:TYR:OH	1:F:949:ASN:ND2	2.37	0.53
1:A:319:ILE:CG2	1:A:677:PRO:HB3	2.39	0.53
1:B:61:LEU:HB3	1:B:75:VAL:HG13	1.91	0.53
1:C:1036:ALA:O	1:C:1039:ASP:HB2	2.09	0.53
1:E:220:GLY:O	1:E:1038:HIS:HB3	2.09	0.53
1:A:676:ARG:NH1	1:D:811:ASP:OD1	2.42	0.53
1:C:190:ARG:NH2	1:C:222:PHE:CZ	2.75	0.53
1:E:568:LEU:HB3	1:E:571:MET:CE	2.39	0.53
1:F:190:ARG:NH2	1:F:222:PHE:HZ	2.07	0.53
1:F:206:ARG:N	1:F:1024:ASN:HD21	2.04	0.53
1:A:156:PHE:HB2	1:A:159:MET:HE2	1.91	0.53
1:A:562:GLU:O	1:A:563:ALA:HB3	2.09	0.53
1:B:546:PRO:HG2	1:B:567:ASP:HB3	1.91	0.53
1:C:82:ASN:HD21	1:C:96:ARG:HD3	1.71	0.53
1:C:524:PRO:HD3	1:D:605:GLU:CG	2.39	0.53
1:F:64:HIS:HD2	1:F:71:THR:OG1	1.91	0.53
1:A:167:ASN:HB2	1:A:170:ILE:HB	1.90	0.53
1:C:46:PRO:HB2	1:C:286:LEU:HD21	1.90	0.53
1:C:722:VAL:N	1:C:723:PRO:HD2	2.24	0.53
1:D:418:PHE:HA	1:D:433:LEU:HG	1.89	0.53
1:F:253:GLN:HB2	1:F:255:TYR:HE1	1.74	0.53
1:F:618:VAL:CG2	1:F:631:GLU:HG3	2.39	0.53
1:A:82:ASN:HD21	1:A:96:ARG:HH21	1.56	0.53
1:A:88:PRO:HG3	1:A:144:GLY:HA2	1.91	0.53
1:C:241:ARG:NH1	1:C:263:ASP:HB3	2.24	0.53
1:C:393:ARG:HH22	1:E:557:ARG:NE	2.07	0.53
1:D:61:LEU:HB3	1:D:75:VAL:HG13	1.90	0.53
1:D:319:ILE:HG23	1:D:677:PRO:HB3	1.91	0.53
1:F:134:PHE:O	1:F:135:THR:HB	2.09	0.53
1:F:700:ASN:HD22	1:F:1008:GLN:NE2	2.07	0.53
1:F:977:LEU:HB2	1:F:979:LEU:CD1	2.39	0.53
1:A:61:LEU:CB	1:A:75:VAL:HG13	2.39	0.52
1:A:423:ASN:ND2	1:A:425:ARG:HB2	2.24	0.52
1:B:337:ILE:HG22	1:B:338:ALA:N	2.24	0.52
1:B:706:VAL:HG12	1:B:710:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:982:LEU:C	1:B:983:ILE:HD12	2.29	0.52
1:C:404:LEU:HD22	1:C:429:MET:CE	2.39	0.52
1:E:295:ILE:HG13	1:E:306:ILE:HD11	1.90	0.52
1:F:249:ASP:HB2	2:F:7014:HOH:O	2.09	0.52
1:F:735:ILE:O	1:F:738:MET:HG3	2.09	0.52
1:A:393:ARG:NH1	1:C:557:ARG:HD2	2.24	0.52
1:C:53:ILE:HD11	1:C:295:ILE:HD11	1.92	0.52
1:D:333:ASP:CG	1:D:369:ARG:HE	2.12	0.52
1:F:1052:ILE:O	1:F:1056:ILE:HG13	2.10	0.52
1:C:716:GLU:HG2	1:C:720:ASN:ND2	2.24	0.52
1:D:179:PRO:HG2	2:D:5045:HOH:O	2.09	0.52
1:D:913:ARG:HH21	1:D:1047:GLN:NE2	2.07	0.52
1:E:524:PRO:HD3	1:F:605:GLU:CG	2.39	0.52
1:B:319:ILE:CG2	1:B:677:PRO:HB3	2.39	0.52
1:E:403:ASN:HD22	1:E:404:LEU:N	2.06	0.52
1:E:642:SER:HB2	1:E:647:THR:HB	1.91	0.52
1:F:729:TYR:O	1:F:732:SER:HB3	2.09	0.52
1:B:155:PRO:HD2	1:B:159:MET:HE3	1.90	0.52
1:C:249:ASP:HB2	2:C:4014:HOH:O	2.08	0.52
1:D:155:PRO:CG	1:D:159:MET:HE1	2.23	0.52
1:B:815:VAL:HA	1:B:819:SER:HB3	1.91	0.52
1:C:308:ILE:HG22	1:C:311:LEU:HD11	1.91	0.52
1:C:333:ASP:CG	1:C:369:ARG:HE	2.13	0.52
1:C:676:ARG:HD2	2:C:4370:HOH:O	2.08	0.52
1:E:781:ALA:HB2	1:E:802:PRO:HG2	1.91	0.52
1:F:123:TYR:OH	1:F:823:ARG:HD3	2.10	0.52
1:F:123:TYR:HB3	1:F:826:SER:OG	2.09	0.52
1:F:593:SER:O	1:F:624:VAL:HG22	2.10	0.52
1:A:190:ARG:NH2	1:A:222:PHE:HZ	2.07	0.52
1:A:982:LEU:C	1:A:983:ILE:HD12	2.30	0.52
1:B:467:LEU:C	1:B:467:LEU:HD12	2.29	0.52
1:D:557:ARG:HD2	1:F:393:ARG:HH12	1.75	0.52
1:A:580:VAL:HG22	1:A:622:TYR:CD2	2.44	0.52
1:B:156:PHE:HB2	1:B:159:MET:HE2	1.92	0.52
1:B:913:ARG:HH21	1:B:1047:GLN:NE2	2.08	0.52
1:C:52:ARG:HG3	1:C:52:ARG:HH21	1.75	0.52
1:C:184:LEU:HD13	1:C:237:ILE:HG13	1.90	0.52
1:C:807:ILE:HG12	1:C:837:LEU:CD2	2.40	0.52
1:E:216:GLU:OE1	1:E:219:SER:HA	2.10	0.52
1:A:781:ALA:HB2	1:A:802:PRO:HG2	1.90	0.52
1:C:350:VAL:CG2	1:C:669:ARG:HH11	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:N	1:A:1024:ASN:HD21	2.07	0.52
1:A:363:ARG:HD2	1:A:365:ARG:NH2	2.25	0.52
1:B:190:ARG:NH2	1:B:222:PHE:CZ	2.77	0.52
1:B:387:LEU:HD13	1:B:388:GLY:N	2.24	0.52
1:D:885:PRO:O	1:D:915:ASN:HA	2.09	0.52
1:A:475:TYR:OH	1:B:949:ASN:ND2	2.43	0.51
1:B:314:PRO:HD2	1:B:726:LYS:HG2	1.92	0.51
1:C:684:GLU:HG3	1:C:685:GLU:N	2.24	0.51
1:D:156:PHE:HD1	1:D:159:MET:CE	2.23	0.51
1:E:684:GLU:HG3	1:E:685:GLU:N	2.24	0.51
1:F:222:PHE:H	1:F:1038:HIS:CD2	2.28	0.51
1:F:651:ARG:NH2	1:F:655:GLY:O	2.42	0.51
1:A:681:SER:CB	1:A:684:GLU:HG2	2.39	0.51
1:B:965:SER:HA	1:B:990:GLY:O	2.10	0.51
1:C:776:TYR:CD1	1:C:816:GLY:HA2	2.45	0.51
1:D:202:TRP:CH2	1:D:745:SER:HB3	2.45	0.51
1:D:562:GLU:O	1:D:563:ALA:HB3	2.10	0.51
1:D:1016:ARG:O	1:D:1017:ASP:HB2	2.10	0.51
1:E:156:PHE:HD1	1:E:159:MET:HE1	1.76	0.51
1:E:578:ILE:CD1	1:E:595:ILE:HD12	2.41	0.51
1:F:241:ARG:NH1	1:F:263:ASP:OD1	2.44	0.51
1:F:1055:LEU:O	1:F:1059:LEU:HD13	2.10	0.51
1:E:889:MET:SD	1:F:522:PRO:HG2	2.50	0.51
1:F:430:THR:HG23	1:F:441:ILE:HD11	1.92	0.51
1:B:222:PHE:H	1:B:1038:HIS:CD2	2.28	0.51
1:C:489:LYS:HG3	1:C:491:PHE:CE1	2.45	0.51
1:C:703:ASN:C	1:C:703:ASN:HD22	2.13	0.51
1:E:155:PRO:HG2	1:E:159:MET:CE	2.32	0.51
1:E:222:PHE:H	1:E:1038:HIS:CD2	2.28	0.51
1:C:893:ASN:OD1	1:D:522:PRO:HD3	2.11	0.51
1:D:130:GLY:HA3	2:D:5163:HOH:O	2.10	0.51
1:E:522:PRO:HG2	1:F:889:MET:SD	2.50	0.51
1:B:393:ARG:HH12	1:F:557:ARG:CD	2.23	0.51
1:B:589:ILE:HD13	1:B:641:LEU:CD1	2.41	0.51
1:C:242:ILE:O	1:C:256:SER:HA	2.10	0.51
1:C:802:PRO:O	1:C:805:TYR:HB2	2.11	0.51
1:F:589:ILE:HG21	1:F:641:LEU:HD11	1.91	0.51
1:C:494:THR:HG21	1:C:500:ASP:OD1	2.11	0.51
1:F:238:VAL:HG11	1:F:298:PRO:HG2	1.93	0.51
1:B:205:TYR:HA	1:B:1024:ASN:HD21	1.76	0.51
1:B:315:GLU:OE2	1:E:119:LYS:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:HD23	1:C:287:PHE:HB3	1.92	0.51
1:C:736:VAL:HA	1:C:739:GLN:HE21	1.76	0.51
1:D:123:TYR:HB3	1:D:826:SER:OG	2.11	0.51
1:A:1031:VAL:HG12	1:A:1033:ILE:CD1	2.40	0.51
1:D:593:SER:O	1:D:624:VAL:HG22	2.11	0.51
1:E:530:ASN:HD22	1:E:531:PHE:H	1.55	0.51
1:F:205:TYR:HA	1:F:1024:ASN:HD21	1.76	0.51
1:B:446:GLU:OE1	1:B:468:LYS:HE2	2.11	0.50
1:C:350:VAL:HG23	1:C:351:SER:N	2.26	0.50
1:E:156:PHE:HD1	1:E:159:MET:CE	2.24	0.50
1:E:700:ASN:HD22	1:E:1008:GLN:NE2	2.09	0.50
1:F:245:ILE:HD11	1:F:278:LEU:HG	1.92	0.50
1:A:43:LEU:HD13	1:A:308:ILE:HD12	1.92	0.50
1:A:134:PHE:O	1:A:135:THR:HB	2.12	0.50
1:B:373:THR:HG21	1:B:393:ARG:HD2	1.92	0.50
1:C:153:MET:HG3	1:C:859:ARG:NH1	2.26	0.50
1:E:703:ASN:C	1:E:703:ASN:HD22	2.13	0.50
1:F:156:PHE:H	1:F:159:MET:CE	2.24	0.50
1:D:676:ARG:HD2	2:D:5370:HOH:O	2.11	0.50
1:F:53:ILE:HG23	1:F:286:LEU:CD2	2.39	0.50
1:F:493:ALA:HA	1:F:571:MET:HG3	1.92	0.50
1:C:709:GLU:OE2	1:C:713:ARG:HD3	2.11	0.50
1:D:236:VAL:HG23	1:D:243:TYR:HB2	1.93	0.50
1:E:46:PRO:HB2	1:E:286:LEU:CD2	2.41	0.50
1:E:578:ILE:HG12	1:E:580:VAL:HG23	1.94	0.50
1:A:156:PHE:CD1	1:A:159:MET:HE1	2.47	0.50
1:B:363:ARG:HG3	1:B:688:GLN:HE22	1.76	0.50
1:B:393:ARG:HH12	1:F:557:ARG:NH2	2.10	0.50
1:D:190:ARG:HH21	1:D:190:ARG:CG	2.24	0.50
1:F:552:THR:HG21	1:F:578:ILE:HD12	1.94	0.50
1:A:48:ILE:HB	1:A:286:LEU:HD22	1.94	0.50
1:B:286:LEU:HD11	1:B:293:ILE:CG2	2.42	0.50
1:C:256:SER:OG	1:C:267:HIS:CE1	2.65	0.50
1:C:317:ARG:HD3	1:F:823:ARG:HD2	1.93	0.50
1:C:206:ARG:H	1:C:1024:ASN:HD21	1.59	0.50
1:C:332:LEU:HD11	1:C:338:ALA:HB2	1.94	0.50
1:C:716:GLU:HG2	1:C:720:ASN:HD21	1.77	0.50
1:E:913:ARG:HH21	1:E:1047:GLN:NE2	2.09	0.50
1:B:872:HIS:CE1	1:B:902:GLU:OE1	2.65	0.50
1:E:618:VAL:HG21	1:E:631:GLU:HG3	1.94	0.50
1:E:694:TRP:HA	1:E:738:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:977:LEU:HB2	1:E:979:LEU:CD1	2.40	0.50
1:F:46:PRO:HB2	1:F:286:LEU:HD21	1.92	0.50
1:A:317:ARG:HD3	1:D:823:ARG:HD2	1.92	0.50
1:C:815:VAL:HA	1:C:819:SER:HB3	1.92	0.50
1:D:557:ARG:NE	1:F:393:ARG:HH22	2.10	0.50
1:F:452:PHE:HB3	1:F:463:TYR:HB3	1.94	0.50
1:A:992:VAL:HG11	1:A:1009:PRO:HB2	1.93	0.49
1:B:403:ASN:HD22	1:B:403:ASN:C	2.16	0.49
1:B:681:SER:O	1:B:684:GLU:HG2	2.12	0.49
1:E:286:LEU:HD13	1:E:295:ILE:HG12	1.94	0.49
1:E:618:VAL:CG2	1:E:631:GLU:HG3	2.41	0.49
1:E:965:SER:HA	1:E:990:GLY:O	2.12	0.49
1:F:333:ASP:CG	1:F:369:ARG:HE	2.14	0.49
1:F:616:LYS:HE2	1:F:653:ASP:CB	2.42	0.49
1:C:228:MET:HE1	1:C:244:PHE:CE1	2.47	0.49
1:C:731:LEU:HD22	1:C:735:ILE:HG13	1.95	0.49
1:C:732:SER:O	1:C:736:VAL:HG23	2.12	0.49
1:D:350:VAL:HG21	1:D:669:ARG:HH11	1.76	0.49
1:E:123:TYR:HB3	1:E:826:SER:OG	2.10	0.49
1:F:177:LEU:HD13	1:F:192:ILE:HD11	1.94	0.49
1:F:639:LEU:HD23	1:F:639:LEU:C	2.33	0.49
1:A:236:VAL:HG23	1:A:243:TYR:HB2	1.93	0.49
1:A:498:SER:OG	1:A:499:HIS:N	2.44	0.49
1:C:218:ASN:O	1:C:221:ALA:N	2.45	0.49
1:C:988:TRP:CZ3	1:C:990:GLY:HA3	2.47	0.49
1:E:300:THR:O	1:E:301:GLU:HB3	2.12	0.49
1:F:346:PHE:C	1:F:347:ILE:HD12	2.32	0.49
1:A:605:GLU:HG2	1:B:524:PRO:HD3	1.93	0.49
1:C:363:ARG:NH2	1:C:365:ARG:HH22	2.11	0.49
1:E:46:PRO:HB2	1:E:286:LEU:HD23	1.94	0.49
1:E:256:SER:OG	1:E:267:HIS:HE1	1.95	0.49
1:A:205:TYR:CE1	1:A:207:GLY:HA3	2.48	0.49
1:A:626:THR:O	1:A:627:ARG:HB2	2.12	0.49
1:B:134:PHE:O	1:B:135:THR:HB	2.12	0.49
1:C:155:PRO:HB3	1:C:860:TYR:HA	1.94	0.49
1:E:736:VAL:HA	1:E:739:GLN:HE21	1.77	0.49
1:A:155:PRO:CD	1:A:159:MET:HE3	2.43	0.49
1:B:104:ASN:HD22	1:B:104:ASN:N	1.93	0.49
1:C:156:PHE:HD1	1:C:159:MET:CE	2.26	0.49
1:D:706:VAL:HG12	1:D:710:ILE:CD1	2.43	0.49
1:D:774:ASP:HA	1:D:817:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HD11	1:B:293:ILE:HG22	1.94	0.49
1:C:218:ASN:O	1:C:219:SER:C	2.50	0.49
1:C:641:LEU:HD22	1:C:645:ARG:HA	1.94	0.49
1:E:346:PHE:C	1:E:347:ILE:HD12	2.33	0.49
1:E:524:PRO:HD3	1:F:605:GLU:HG2	1.94	0.49
1:F:716:GLU:HG2	1:F:720:ASN:ND2	2.27	0.49
1:C:884:ILE:HD13	1:C:924:ILE:HD13	1.94	0.49
1:D:206:ARG:N	1:D:1024:ASN:HD21	2.09	0.49
1:D:618:VAL:CG2	1:D:631:GLU:HG3	2.42	0.49
1:B:350:VAL:CG2	1:B:669:ARG:HH11	2.23	0.49
1:C:141:ASP:HB2	1:C:142:PRO:HD2	1.93	0.49
1:D:167:ASN:HB2	1:D:170:ILE:HB	1.94	0.49
1:D:268:THR:CG2	1:D:303:ILE:HD11	2.40	0.49
1:E:589:ILE:HG21	1:E:641:LEU:HD11	1.95	0.49
1:F:189:ARG:HD2	1:F:216:GLU:O	2.13	0.49
1:F:994:ILE:HG22	1:F:1008:GLN:O	2.13	0.49
1:A:589:ILE:HD13	1:A:641:LEU:HD12	1.95	0.49
1:B:156:PHE:HD1	1:B:159:MET:CE	2.26	0.49
1:D:1033:ILE:HD11	1:D:1050:TYR:CD2	2.48	0.49
1:E:400:PHE:CD2	1:E:436:GLY:HA3	2.48	0.48
1:F:256:SER:OG	1:F:267:HIS:CE1	2.65	0.48
1:A:286:LEU:HD11	1:A:293:ILE:CG2	2.42	0.48
1:B:580:VAL:HG22	1:B:622:TYR:CD2	2.48	0.48
1:D:367:VAL:CG1	1:D:375:VAL:HG21	2.43	0.48
1:E:965:SER:N	1:E:968:ASP:OD2	2.43	0.48
1:A:882:ILE:HD11	1:A:899:PHE:HA	1.94	0.48
1:C:337:ILE:HG22	1:C:338:ALA:N	2.28	0.48
1:C:639:LEU:HD23	1:C:639:LEU:C	2.33	0.48
1:E:499:HIS:HD2	2:E:6176:HOH:O	1.95	0.48
1:E:577:PRO:HG3	1:F:789:GLU:HG3	1.95	0.48
1:F:722:VAL:N	1:F:723:PRO:HD2	2.29	0.48
1:F:890:MET:O	1:F:894:GLU:HG2	2.12	0.48
1:A:578:ILE:HG12	1:A:580:VAL:HG23	1.94	0.48
1:A:676:ARG:HD2	2:A:2370:HOH:O	2.13	0.48
1:B:709:GLU:OE2	1:B:713:ARG:HD3	2.14	0.48
1:D:468:LYS:CD	1:D:473:ASP:HB2	2.38	0.48
1:F:213:ILE:HB	1:F:226:VAL:HB	1.95	0.48
1:F:706:VAL:HG12	1:F:710:ILE:CD1	2.42	0.48
1:A:155:PRO:CG	1:A:159:MET:HE1	2.31	0.48
1:A:977:LEU:HB2	1:A:979:LEU:HD13	1.96	0.48
1:A:1016:ARG:O	1:A:1017:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:CD1	1:B:306:ILE:HD13	2.42	0.48
1:C:977:LEU:HB2	1:C:979:LEU:HD13	1.95	0.48
1:F:897:ARG:HG2	1:F:898:LEU:HD12	1.96	0.48
1:B:524:PRO:HB3	1:B:531:PHE:CE2	2.49	0.48
1:C:119:LYS:NZ	1:C:823:ARG:HH22	2.12	0.48
1:C:205:TYR:HA	1:C:1024:ASN:HD21	1.77	0.48
1:C:929:MET:HA	1:C:929:MET:HE3	1.95	0.48
1:A:499:HIS:HD2	2:A:2176:HOH:O	1.95	0.48
1:B:639:LEU:C	1:B:639:LEU:HD23	2.34	0.48
1:E:167:ASN:O	1:E:170:ILE:HG12	2.13	0.48
1:E:802:PRO:O	1:E:805:TYR:HB2	2.13	0.48
1:F:284:ARG:HD3	2:F:7393:HOH:O	2.13	0.48
1:F:309:GLY:O	1:F:311:LEU:HD13	2.14	0.48
1:A:791:GLU:CD	1:A:861:ARG:HE	2.16	0.48
1:B:505:PHE:CE2	1:B:512:LEU:HD13	2.48	0.48
1:C:78:LEU:HB2	2:C:4254:HOH:O	2.13	0.48
1:C:238:VAL:HG11	1:C:298:PRO:HG2	1.94	0.48
1:C:241:ARG:HB2	1:C:243:TYR:HE1	1.79	0.48
1:C:735:ILE:O	1:C:739:GLN:HG3	2.13	0.48
1:D:430:THR:HG23	1:D:441:ILE:HD11	1.96	0.48
1:A:218:ASN:HB3	1:A:221:ALA:HB3	1.95	0.48
1:E:999:ARG:HG2	1:E:1005:VAL:HG22	1.95	0.48
1:A:556:PRO:HD3	1:E:354:TYR:CD1	2.49	0.48
1:B:230:THR:HG21	1:B:248:ILE:HA	1.95	0.48
1:B:425:ARG:O	1:B:426:PHE:HB2	2.14	0.48
1:B:562:GLU:O	1:B:563:ALA:HB3	2.14	0.48
1:C:605:GLU:HG2	1:D:524:PRO:HD3	1.95	0.48
1:E:53:ILE:CD1	1:E:306:ILE:HD13	2.44	0.48
1:E:983:ILE:HG23	1:E:1033:ILE:CD1	2.38	0.48
1:B:498:SER:HB2	2:B:2192:HOH:O	2.13	0.47
1:C:48:ILE:HG12	1:C:49:HIS:N	2.28	0.47
1:C:297:ASN:O	1:C:301:GLU:N	2.44	0.47
1:C:681:SER:CB	1:C:684:GLU:HG2	2.42	0.47
1:D:425:ARG:O	1:D:426:PHE:HB2	2.13	0.47
1:D:913:ARG:NH2	1:D:1047:GLN:HE21	2.10	0.47
1:F:403:ASN:HD22	1:F:404:LEU:N	2.12	0.47
1:A:53:ILE:CD1	1:A:306:ILE:HD13	2.45	0.47
1:B:360:GLU:HB2	1:B:364:ILE:HD11	1.97	0.47
1:D:228:MET:HE1	1:D:232:VAL:HG22	1.96	0.47
1:E:155:PRO:CG	1:E:159:MET:HE1	2.35	0.47
1:E:194:ARG:O	1:E:211:GLY:HA2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:578:ILE:HD12	1:E:595:ILE:HD12	1.96	0.47
1:A:314:PRO:HD2	1:A:726:LYS:HG2	1.94	0.47
1:F:681:SER:HB3	1:F:684:GLU:HG2	1.97	0.47
1:A:63:GLU:OE1	1:A:72:ARG:NH1	2.48	0.47
1:A:270:PHE:CD2	1:A:289:LYS:HE2	2.50	0.47
1:A:337:ILE:HD11	1:A:350:VAL:HG12	1.95	0.47
1:B:355:VAL:CG1	1:B:676:ARG:HH21	2.26	0.47
1:C:64:HIS:HD2	1:C:71:THR:OG1	1.97	0.47
1:C:956:ILE:HG22	1:C:1055:LEU:HD11	1.96	0.47
1:E:565:GLU:HG2	1:E:566:TYR:N	2.28	0.47
1:F:218:ASN:O	1:F:221:ALA:N	2.48	0.47
1:A:393:ARG:HH12	1:C:557:ARG:CD	2.25	0.47
1:C:110:PHE:CD2	1:C:121:ILE:HG13	2.50	0.47
1:C:231:HIS:HD2	2:C:4052:HOH:O	1.97	0.47
1:C:236:VAL:CG2	1:C:243:TYR:HB2	2.44	0.47
1:C:253:GLN:HB2	1:C:255:TYR:CE1	2.49	0.47
1:D:872:HIS:CE1	1:D:902:GLU:OE1	2.66	0.47
1:F:319:ILE:CG2	1:F:677:PRO:HB3	2.44	0.47
1:A:349:ASP:OD2	1:A:353:THR:HG22	2.15	0.47
1:B:43:LEU:HD13	1:B:308:ILE:HD12	1.96	0.47
1:B:1016:ARG:O	1:B:1017:ASP:HB2	2.13	0.47
1:C:425:ARG:O	1:C:426:PHE:HB2	2.15	0.47
1:C:537:SER:HB3	1:C:583:GLY:O	2.15	0.47
1:C:949:ASN:ND2	1:D:475:TYR:OH	2.40	0.47
1:D:350:VAL:CG2	1:D:669:ARG:HH11	2.27	0.47
1:E:493:ALA:HA	1:E:571:MET:HG3	1.96	0.47
1:E:701:TYR:O	1:F:939:ARG:HD3	2.14	0.47
1:A:155:PRO:HG2	1:A:159:MET:CE	2.30	0.47
1:A:309:GLY:O	1:A:311:LEU:HD13	2.14	0.47
1:A:327:GLU:O	1:A:328:ASP:C	2.53	0.47
1:A:401:GLU:OE2	1:A:401:GLU:N	2.43	0.47
1:B:53:ILE:HD11	1:B:295:ILE:HD11	1.95	0.47
1:B:736:VAL:HA	1:B:739:GLN:HE21	1.79	0.47
1:C:218:ASN:HB3	1:C:221:ALA:HB3	1.97	0.47
1:C:982:LEU:C	1:C:983:ILE:HD12	2.35	0.47
1:E:110:PHE:CD2	1:E:121:ILE:HG13	2.50	0.47
1:E:228:MET:HE1	1:E:244:PHE:CE1	2.49	0.47
1:E:293:ILE:CG2	1:E:306:ILE:HD12	2.45	0.47
1:F:442:GLU:OE2	1:F:481:HIS:HD2	1.98	0.47
1:F:791:GLU:CD	1:F:861:ARG:HE	2.18	0.47
1:B:557:ARG:NH2	1:D:393:ARG:HH12	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LEU:HD11	1:C:293:ILE:HG22	1.96	0.47
1:E:319:ILE:HG23	1:E:677:PRO:HB3	1.96	0.47
1:E:425:ARG:O	1:E:426:PHE:HB2	2.15	0.47
1:F:537:SER:HB3	1:F:583:GLY:O	2.15	0.47
1:A:43:LEU:CD1	1:A:308:ILE:HD12	2.45	0.47
1:B:61:LEU:HB3	1:B:75:VAL:CG1	2.45	0.47
1:B:367:VAL:CG1	1:B:375:VAL:HG21	2.44	0.47
1:D:293:ILE:HG22	1:D:306:ILE:HD12	1.97	0.47
1:D:651:ARG:NH2	1:D:655:GLY:O	2.41	0.47
1:A:156:PHE:HD1	1:A:159:MET:CE	2.27	0.47
1:C:578:ILE:CG1	1:C:580:VAL:HG23	2.43	0.47
1:C:939:ARG:HD3	1:D:701:TYR:O	2.14	0.47
1:D:74:ILE:HG13	1:D:75:VAL:HG12	1.96	0.47
1:E:562:GLU:O	1:E:563:ALA:HB3	2.15	0.47
1:A:190:ARG:CG	1:A:190:ARG:HH21	2.28	0.46
1:A:205:TYR:CZ	1:A:207:GLY:HA3	2.50	0.46
1:A:623:ASP:O	1:A:627:ARG:N	2.47	0.46
1:C:328:ASP:O	1:C:339:PHE:HA	2.14	0.46
1:C:676:ARG:NH1	1:F:811:ASP:OD1	2.48	0.46
1:C:758:ASP:HB3	2:C:4314:HOH:O	2.15	0.46
1:C:493:ALA:HA	1:C:571:MET:HG3	1.96	0.46
1:C:1016:ARG:O	1:C:1017:ASP:HB2	2.15	0.46
1:E:203:LYS:HG2	1:E:274:TYR:CZ	2.50	0.46
1:E:501:TYR:N	1:E:501:TYR:CD2	2.82	0.46
1:A:337:ILE:HG22	1:A:338:ALA:N	2.31	0.46
1:A:949:ASN:ND2	1:B:475:TYR:OH	2.47	0.46
1:C:46:PRO:CG	1:C:286:LEU:HG	2.45	0.46
1:C:430:THR:HG23	1:C:441:ILE:HD11	1.97	0.46
1:E:373:THR:HG21	1:E:393:ARG:HD2	1.96	0.46
1:E:591:LEU:CD1	1:E:662:LEU:HD21	2.43	0.46
1:F:820:ASN:O	1:F:824:VAL:HG23	2.14	0.46
1:A:393:ARG:NH1	1:C:557:ARG:NH2	2.62	0.46
1:D:222:PHE:H	1:D:1038:HIS:CD2	2.34	0.46
1:E:195:ASN:O	1:E:231:HIS:HE1	1.98	0.46
1:E:268:THR:CG2	1:E:303:ILE:HD11	2.41	0.46
1:F:642:SER:HB3	1:F:647:THR:H	1.80	0.46
1:F:781:ALA:HB2	1:F:802:PRO:HG2	1.97	0.46
1:B:220:GLY:O	1:B:1038:HIS:HB3	2.15	0.46
1:C:92:LYS:HD3	1:C:110:PHE:CD1	2.50	0.46
1:C:860:TYR:OH	1:C:885:PRO:HD3	2.14	0.46
1:D:222:PHE:H	1:D:1038:HIS:HD2	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:LEU:HD22	1:D:735:ILE:HG13	1.97	0.46
1:D:986:ARG:HD3	1:D:1028:ASP:OD2	2.16	0.46
1:E:550:ASN:HB3	1:E:553:LYS:HG3	1.96	0.46
1:A:511:ASN:ND2	1:A:543:PRO:HA	2.30	0.46
1:A:872:HIS:CE1	1:A:902:GLU:OE1	2.67	0.46
1:B:393:ARG:HH12	1:F:557:ARG:NE	2.14	0.46
1:E:423:ASN:C	1:E:423:ASN:HD22	2.18	0.46
1:F:463:TYR:CE1	1:F:481:HIS:HB2	2.51	0.46
1:F:589:ILE:HB	1:F:596:LEU:HB2	1.96	0.46
1:A:110:PHE:HE2	1:A:146:LEU:HD22	1.81	0.46
1:A:167:ASN:O	1:A:170:ILE:HG12	2.15	0.46
1:C:580:VAL:HG22	1:C:622:TYR:CD2	2.51	0.46
1:D:300:THR:O	1:D:301:GLU:HB3	2.16	0.46
1:D:1014:TRP:HB2	1:D:1020:PHE:CE2	2.50	0.46
1:F:511:ASN:HD22	1:F:543:PRO:HA	1.81	0.46
1:A:228:MET:HE1	1:A:244:PHE:CE1	2.51	0.46
1:A:618:VAL:CG2	1:A:631:GLU:HG3	2.46	0.46
1:A:992:VAL:CG1	1:A:1009:PRO:HB2	2.46	0.46
1:B:228:MET:HE1	1:B:244:PHE:CE1	2.51	0.46
1:B:700:ASN:HD22	1:B:1008:GLN:NE2	2.12	0.46
1:C:596:LEU:N	1:C:596:LEU:CD2	2.78	0.46
1:C:641:LEU:HD23	1:C:642:SER:H	1.81	0.46
1:E:53:ILE:HD12	1:E:306:ILE:HD13	1.97	0.46
1:E:929:MET:CE	1:E:929:MET:HA	2.46	0.46
1:A:355:VAL:HG12	1:A:676:ARG:HH21	1.81	0.46
1:A:425:ARG:O	1:A:426:PHE:HB2	2.16	0.46
1:A:639:LEU:HD23	1:A:639:LEU:C	2.36	0.46
1:B:565:GLU:HG2	1:B:566:TYR:N	2.30	0.46
1:B:591:LEU:CD1	1:B:662:LEU:HD21	2.46	0.46
1:B:641:LEU:HD23	1:B:642:SER:H	1.80	0.46
1:C:855:ASP:HA	2:C:4221:HOH:O	2.16	0.46
1:C:892:LEU:HD13	1:C:920:VAL:HG21	1.96	0.46
1:E:735:ILE:O	1:E:739:GLN:HG3	2.16	0.46
1:E:123:TYR:OH	1:E:823:ARG:HD3	2.15	0.46
1:E:992:VAL:HG11	1:E:1009:PRO:HB2	1.98	0.46
1:E:997:LYS:NZ	2:E:7168:HOH:O	2.47	0.46
1:F:190:ARG:NH2	1:F:222:PHE:CZ	2.84	0.46
1:F:423:ASN:ND2	1:F:425:ARG:HB2	2.32	0.46
1:F:511:ASN:ND2	1:F:543:PRO:HA	2.30	0.46
1:A:403:ASN:HD22	1:A:403:ASN:C	2.18	0.45
1:A:807:ILE:HG12	1:A:837:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:GLU:OE1	1:A:1034:GLU:OE2	2.34	0.45
1:B:156:PHE:CD1	1:B:159:MET:HE1	2.52	0.45
1:B:442:GLU:OE2	1:B:481:HIS:HD2	1.97	0.45
1:D:190:ARG:HH21	1:D:190:ARG:CB	2.28	0.45
1:D:387:LEU:HD13	1:D:388:GLY:N	2.31	0.45
1:E:218:ASN:O	1:E:220:GLY:N	2.49	0.45
1:E:368:ARG:O	1:E:375:VAL:HG23	2.16	0.45
1:E:562:GLU:HB3	1:E:563:ALA:H	1.60	0.45
1:E:706:VAL:HG12	1:E:710:ILE:CD1	2.46	0.45
1:E:897:ARG:HG2	1:E:898:LEU:HD12	1.98	0.45
1:F:369:ARG:HH21	1:F:369:ARG:HG3	1.79	0.45
1:F:959:THR:O	1:F:984:GLY:HA3	2.15	0.45
1:A:418:PHE:HA	1:A:433:LEU:HG	1.98	0.45
1:B:195:ASN:O	1:B:231:HIS:HE1	1.99	0.45
1:B:369:ARG:HD2	1:B:371:GLY:H	1.80	0.45
1:B:579:ASN:ND2	1:B:627:ARG:NH1	2.64	0.45
1:D:528:VAL:HG12	1:D:529:LEU:N	2.31	0.45
1:E:61:LEU:HD13	1:E:74:ILE:HD11	1.97	0.45
1:E:228:MET:HE1	1:E:232:VAL:HG22	1.98	0.45
1:E:418:PHE:HA	1:E:433:LEU:HG	1.98	0.45
1:A:1055:LEU:O	1:A:1059:LEU:HD13	2.16	0.45
1:B:578:ILE:CD1	1:B:595:ILE:HD12	2.46	0.45
1:C:681:SER:HB3	1:C:684:GLU:CG	2.45	0.45
1:D:906:GLN:O	1:D:953:GLY:HA3	2.16	0.45
1:E:589:ILE:HB	1:E:596:LEU:HB2	1.97	0.45
1:A:57:CYS:HB3	1:A:62:TRP:CD1	2.51	0.45
1:A:156:PHE:HD1	1:A:159:MET:HE1	1.81	0.45
1:A:249:ASP:HB2	2:A:2014:HOH:O	2.16	0.45
1:A:347:ILE:HD12	1:A:347:ILE:N	2.32	0.45
1:A:369:ARG:HD2	1:A:371:GLY:H	1.81	0.45
1:D:373:THR:HG21	1:D:393:ARG:HD2	1.98	0.45
1:D:402:GLU:HG3	1:D:438:PRO:HD3	1.98	0.45
1:E:528:VAL:HG12	1:E:529:LEU:N	2.31	0.45
1:E:596:LEU:HD22	1:E:596:LEU:N	2.31	0.45
1:E:790:GLY:HA2	2:E:6244:HOH:O	2.17	0.45
1:F:136:ASP:OD2	1:F:137:VAL:N	2.42	0.45
1:F:580:VAL:HG22	1:F:622:TYR:CD2	2.52	0.45
1:B:393:ARG:NH1	1:F:557:ARG:HD2	2.32	0.45
1:C:589:ILE:HD13	1:C:641:LEU:HD12	1.99	0.45
1:C:886:ASP:O	1:C:891:GLY:HA3	2.17	0.45
1:D:232:VAL:HG13	1:D:244:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:641:LEU:HD22	1:E:645:ARG:HA	1.98	0.45
1:D:44:LEU:HD22	1:D:733:ASN:ND2	2.32	0.45
1:D:690:TYR:CE2	1:D:719:ARG:HB2	2.52	0.45
1:F:1016:ARG:O	1:F:1017:ASP:HB2	2.16	0.45
1:B:53:ILE:HD13	1:B:306:ILE:HD13	1.98	0.45
1:C:781:ALA:HB2	1:C:802:PRO:HG2	1.98	0.45
1:E:619:LEU:HD13	1:E:639:LEU:CD1	2.47	0.45
1:B:63:GLU:OE1	1:B:72:ARG:NH1	2.50	0.45
1:B:977:LEU:HB2	1:B:979:LEU:CD1	2.47	0.45
1:D:537:SER:HB3	1:D:583:GLY:O	2.17	0.45
1:E:893:ASN:OD1	1:F:522:PRO:HD3	2.16	0.45
1:E:1033:ILE:HD11	1:E:1050:TYR:CD2	2.51	0.45
1:C:642:SER:HB2	1:C:647:THR:HB	1.99	0.45
1:E:467:LEU:HD12	1:E:467:LEU:C	2.37	0.45
1:A:393:ARG:HH12	1:C:557:ARG:CZ	2.30	0.45
1:A:430:THR:HG23	1:A:441:ILE:HD11	1.99	0.45
1:A:565:GLU:HG2	1:A:566:TYR:N	2.32	0.45
1:A:591:LEU:CD1	1:A:596:LEU:HD23	2.47	0.45
1:C:463:TYR:CE1	1:C:481:HIS:HB2	2.52	0.45
1:D:235:PRO:HA	1:D:243:TYR:O	2.17	0.45
1:E:360:GLU:HB2	1:E:364:ILE:HD11	1.99	0.45
1:E:885:PRO:O	1:E:915:ASN:HA	2.17	0.45
1:F:141:ASP:HB2	1:F:142:PRO:HD2	1.98	0.45
1:F:300:THR:HG22	1:F:300:THR:O	2.16	0.45
1:F:860:TYR:CZ	1:F:864:VAL:HG21	2.52	0.45
1:A:195:ASN:O	1:A:231:HIS:HE1	2.00	0.44
1:A:929:MET:HA	1:A:929:MET:CE	2.47	0.44
1:B:295:ILE:CG1	1:B:306:ILE:HD11	2.41	0.44
1:B:309:GLY:O	1:B:311:LEU:HD13	2.18	0.44
1:C:642:SER:HB3	1:C:647:THR:H	1.82	0.44
1:D:736:VAL:HA	1:D:739:GLN:HE21	1.82	0.44
1:F:912:VAL:O	1:F:915:ASN:HB2	2.17	0.44
1:A:403:ASN:HD22	1:A:404:LEU:N	2.16	0.44
1:B:441:ILE:HG23	1:B:483:TYR:CD1	2.52	0.44
1:C:82:ASN:ND2	1:C:96:ARG:HH21	2.14	0.44
1:C:279:ASN:HD22	1:C:279:ASN:HA	1.63	0.44
1:C:308:ILE:CG2	1:C:311:LEU:HD11	2.47	0.44
1:F:47:ASP:OD1	1:F:85:ARG:HA	2.17	0.44
1:F:321:ILE:HB	1:F:324:LYS:HG3	1.99	0.44
1:F:731:LEU:HD22	1:F:735:ILE:CD1	2.47	0.44
1:A:228:MET:HE1	1:A:232:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LEU:CD2	1:B:645:ARG:HA	2.48	0.44
1:D:681:SER:HB3	1:D:684:GLU:CG	2.47	0.44
1:D:722:VAL:N	1:D:723:PRO:HD2	2.33	0.44
1:E:213:ILE:HB	1:E:226:VAL:HB	1.99	0.44
1:E:367:VAL:HG13	1:E:375:VAL:HG21	1.97	0.44
1:B:988:TRP:CZ3	1:B:990:GLY:HA3	2.52	0.44
1:D:319:ILE:HA	1:D:678:LEU:O	2.18	0.44
1:E:387:LEU:HD13	1:E:388:GLY:N	2.32	0.44
1:E:989:GLY:HA2	1:E:1026:GLY:HA2	2.00	0.44
1:A:404:LEU:HD22	1:A:429:MET:CE	2.42	0.44
1:A:624:VAL:HG23	1:A:625:LYS:N	2.33	0.44
1:B:91:ARG:NH2	1:B:114:GLU:OE1	2.50	0.44
1:B:681:SER:HB3	1:B:684:GLU:CG	2.44	0.44
1:B:1031:VAL:O	1:B:1033:ILE:HD12	2.17	0.44
1:C:130:GLY:HA3	2:C:4163:HOH:O	2.17	0.44
1:C:203:LYS:O	1:C:743:ARG:HG2	2.17	0.44
1:C:403:ASN:HD22	1:C:404:LEU:N	2.15	0.44
1:D:530:ASN:HD22	1:D:531:PHE:H	1.66	0.44
1:D:781:ALA:HB2	1:D:802:PRO:HG2	1.98	0.44
1:E:347:ILE:HD12	1:E:347:ILE:N	2.31	0.44
1:F:45:ASN:N	1:F:45:ASN:ND2	2.64	0.44
1:F:228:MET:HE1	1:F:244:PHE:CE1	2.53	0.44
1:F:738:MET:SD	1:F:738:MET:C	2.96	0.44
1:A:557:ARG:CZ	1:E:393:ARG:HH22	2.31	0.44
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	2.16	0.44
1:A:986:ARG:HD3	1:A:1028:ASP:OD2	2.16	0.44
1:B:327:GLU:O	1:B:328:ASP:O	2.35	0.44
1:B:501:TYR:N	1:B:501:TYR:CD2	2.85	0.44
1:B:890:MET:O	1:B:894:GLU:HG2	2.16	0.44
1:C:289:LYS:HA	2:C:4095:HOH:O	2.17	0.44
1:C:515:LEU:HD23	1:C:539:PRO:HA	1.99	0.44
1:C:651:ARG:NH2	1:C:655:GLY:O	2.46	0.44
1:E:253:GLN:NE2	1:E:268:THR:OG1	2.48	0.44
1:E:452:PHE:HB3	1:E:463:TYR:HB3	2.00	0.44
1:F:350:VAL:CG2	1:F:669:ARG:NH1	2.80	0.44
1:A:82:ASN:HD21	1:A:96:ARG:HD3	1.82	0.44
1:D:190:ARG:HH22	1:D:216:GLU:CD	2.21	0.44
1:D:218:ASN:O	1:D:220:GLY:N	2.50	0.44
1:D:618:VAL:HG21	1:D:631:GLU:HG3	1.98	0.44
1:E:45:ASN:N	1:E:45:ASN:ND2	2.65	0.44
1:E:694:TRP:HA	1:E:738:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ARG:NH2	2:F:7157:HOH:O	2.50	0.44
1:F:253:GLN:HE21	1:F:253:GLN:HA	1.83	0.44
1:F:578:ILE:CD1	1:F:595:ILE:HD12	2.47	0.44
1:A:618:VAL:HG21	1:A:631:GLU:HG3	1.99	0.44
1:A:622:TYR:OH	1:A:627:ARG:HG2	2.18	0.44
1:A:834:ARG:HG3	1:A:846:ASP:OD2	2.18	0.44
1:B:735:ILE:O	1:B:739:GLN:HG3	2.18	0.44
1:C:179:PRO:HG2	2:C:4045:HOH:O	2.16	0.44
1:C:247:ASP:HA	1:C:251:PHE:O	2.18	0.44
1:C:363:ARG:HH21	1:C:365:ARG:HH22	1.64	0.44
1:C:579:ASN:ND2	1:C:627:ARG:NH1	2.66	0.44
1:D:642:SER:HB3	1:D:647:THR:H	1.83	0.44
1:E:104:ASN:ND2	1:E:104:ASN:N	2.62	0.44
1:F:308:ILE:HG22	1:F:311:LEU:CD1	2.48	0.44
1:F:480:ILE:N	1:F:494:THR:HG22	2.20	0.44
1:F:501:TYR:N	1:F:501:TYR:CD2	2.86	0.44
1:F:913:ARG:HH21	1:F:1047:GLN:NE2	2.15	0.44
1:A:53:ILE:HD13	1:A:306:ILE:CD1	2.48	0.44
1:A:218:ASN:O	1:A:219:SER:C	2.55	0.44
1:A:253:GLN:HE22	1:A:270:PHE:N	2.03	0.44
1:A:350:VAL:CG2	1:A:669:ARG:HH11	2.27	0.44
1:A:429:MET:HE3	1:A:438:PRO:CB	2.48	0.44
1:B:393:ARG:NH1	1:F:557:ARG:CZ	2.80	0.44
1:B:499:HIS:HE1	2:B:3239:HOH:O	2.00	0.44
1:B:623:ASP:O	1:B:627:ARG:N	2.50	0.44
1:C:57:CYS:HB3	1:C:62:TRP:NE1	2.33	0.44
1:C:142:PRO:HD3	1:C:185:PHE:CD2	2.53	0.44
1:C:284:ARG:HD3	2:C:4393:HOH:O	2.16	0.44
1:E:218:ASN:O	1:E:219:SER:C	2.56	0.44
1:E:514:TYR:CZ	1:E:540:PHE:HB2	2.53	0.44
1:B:390:TYR:CD1	1:B:397:ALA:HB2	2.53	0.43
1:B:994:ILE:HG22	1:B:1008:GLN:O	2.18	0.43
1:C:218:ASN:O	1:C:220:GLY:N	2.51	0.43
1:E:61:LEU:HB2	1:E:75:VAL:HG13	2.00	0.43
1:F:776:TYR:CD1	1:F:816:GLY:HA2	2.53	0.43
1:A:123:TYR:HB3	1:A:826:SER:OG	2.17	0.43
1:A:1031:VAL:CG1	1:A:1033:ILE:HD11	2.48	0.43
1:B:170:ILE:HD13	1:B:820:ASN:HB2	2.00	0.43
1:B:556:PRO:HD3	1:D:354:TYR:CD1	2.53	0.43
1:C:729:TYR:O	1:C:732:SER:HB3	2.19	0.43
1:C:1014:TRP:CD1	1:C:1019:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ILE:HD12	1:D:347:ILE:N	2.33	0.43
1:D:525:ASP:HB3	1:D:528:VAL:O	2.18	0.43
1:E:89:ASP:CG	1:E:91:ARG:HG3	2.38	0.43
1:E:363:ARG:HG3	1:E:688:GLN:NE2	2.33	0.43
1:E:639:LEU:C	1:E:639:LEU:HD23	2.39	0.43
1:B:82:ASN:HD21	1:B:96:ARG:HD3	1.84	0.43
1:C:965:SER:C	1:C:967:GLY:N	2.71	0.43
1:D:218:ASN:O	1:D:219:SER:C	2.57	0.43
1:D:639:LEU:C	1:D:639:LEU:HD23	2.38	0.43
1:D:791:GLU:CD	1:D:861:ARG:HE	2.21	0.43
1:E:189:ARG:HD2	1:E:216:GLU:O	2.18	0.43
1:F:53:ILE:HD13	1:F:306:ILE:CD1	2.49	0.43
1:F:141:ASP:HB2	1:F:142:PRO:CD	2.48	0.43
1:F:220:GLY:O	1:F:1038:HIS:HB3	2.19	0.43
1:F:882:ILE:HD11	1:F:899:PHE:HA	2.00	0.43
1:A:53:ILE:HD13	1:A:306:ILE:HD13	2.01	0.43
1:A:190:ARG:NH2	1:A:222:PHE:CZ	2.87	0.43
1:A:401:GLU:H	1:A:401:GLU:CD	2.20	0.43
1:A:638:ASP:HB3	1:A:651:ARG:HB3	2.00	0.43
1:C:286:LEU:HD11	1:C:293:ILE:CG2	2.49	0.43
1:C:308:ILE:HG22	1:C:311:LEU:CD1	2.48	0.43
1:C:373:THR:HG21	1:C:393:ARG:HD2	2.00	0.43
1:D:43:LEU:HD13	1:D:308:ILE:HD12	2.01	0.43
1:D:195:ASN:O	1:D:231:HIS:HE1	2.01	0.43
1:D:466:PRO:HB3	2:D:5183:HOH:O	2.17	0.43
1:E:190:ARG:HH21	1:E:190:ARG:CG	2.30	0.43
1:A:142:PRO:HD3	1:A:185:PHE:CD2	2.53	0.43
1:B:314:PRO:HD2	1:B:726:LYS:CG	2.48	0.43
1:E:177:LEU:HD13	1:E:192:ILE:HD11	2.00	0.43
1:E:949:ASN:HB2	2:F:7075:HOH:O	2.18	0.43
1:F:184:LEU:HB2	1:F:191:VAL:HB	2.00	0.43
1:F:337:ILE:HG22	1:F:338:ALA:N	2.33	0.43
1:F:706:VAL:O	1:F:710:ILE:HG13	2.19	0.43
1:A:557:ARG:CZ	1:E:393:ARG:HH12	2.29	0.43
1:A:628:LYS:HE2	1:A:628:LYS:HB3	1.88	0.43
1:B:436:GLY:O	1:B:438:PRO:HD3	2.18	0.43
1:C:528:VAL:HG21	1:C:896:TYR:CD2	2.53	0.43
1:C:872:HIS:CE1	1:C:902:GLU:OE1	2.67	0.43
1:D:530:ASN:ND2	1:D:531:PHE:N	2.64	0.43
1:D:905:TYR:HB2	2:D:5042:HOH:O	2.18	0.43
1:E:489:LYS:HG3	1:E:491:PHE:HE1	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:ASN:HB3	1:F:221:ALA:HB3	1.99	0.43
1:F:442:GLU:OE2	1:F:490:ILE:HD13	2.18	0.43
1:F:802:PRO:O	1:F:805:TYR:HB2	2.18	0.43
1:A:706:VAL:HG12	1:A:710:ILE:CD1	2.49	0.43
1:B:552:THR:HG21	1:B:578:ILE:HD12	2.00	0.43
1:B:637:THR:OG1	1:B:651:ARG:HG3	2.19	0.43
1:D:501:TYR:N	1:D:501:TYR:CD2	2.86	0.43
1:E:61:LEU:HB3	1:E:75:VAL:CG1	2.49	0.43
1:E:319:ILE:HA	1:E:678:LEU:O	2.19	0.43
1:E:616:LYS:HE2	1:E:653:ASP:CB	2.49	0.43
1:E:906:GLN:O	1:E:953:GLY:HA3	2.19	0.43
1:F:319:ILE:HA	1:F:678:LEU:O	2.19	0.43
1:F:389:ILE:HD11	1:F:433:LEU:HB3	2.00	0.43
1:A:333:ASP:CG	1:A:369:ARG:HE	2.22	0.43
1:B:400:PHE:CD2	1:B:436:GLY:HA3	2.54	0.43
1:C:53:ILE:HD13	1:C:306:ILE:CD1	2.48	0.43
1:C:312:GLU:HG2	1:C:314:PRO:HD3	2.00	0.43
1:D:157:SER:HB3	1:D:856:ARG:NH1	2.34	0.43
1:D:771:LEU:HD13	1:D:771:LEU:C	2.39	0.43
1:D:982:LEU:C	1:D:983:ILE:HD12	2.39	0.43
1:E:774:ASP:HA	1:E:817:ALA:HB2	2.00	0.43
1:F:546:PRO:HG2	1:F:567:ASP:HB3	1.99	0.43
1:F:780:LYS:HD3	1:F:782:TYR:CZ	2.54	0.43
1:A:61:LEU:CB	1:A:75:VAL:CG1	2.96	0.43
1:A:61:LEU:HB3	1:A:75:VAL:CG1	2.49	0.43
1:A:190:ARG:NH2	1:A:190:ARG:HG3	2.34	0.43
1:B:327:GLU:O	1:B:328:ASP:C	2.57	0.43
1:C:119:LYS:NZ	1:C:823:ARG:NH2	2.67	0.43
1:C:498:SER:HB2	2:C:5192:HOH:O	2.18	0.43
1:C:622:TYR:OH	1:C:627:ARG:HG2	2.19	0.43
1:D:337:ILE:HG22	1:D:338:ALA:N	2.34	0.43
1:D:400:PHE:CD2	1:D:436:GLY:HA3	2.53	0.43
1:D:965:SER:N	1:D:968:ASP:OD2	2.50	0.43
1:E:651:ARG:NH2	1:E:655:GLY:O	2.46	0.43
1:F:194:ARG:O	1:F:211:GLY:HA2	2.18	0.43
1:A:43:LEU:C	1:A:44:LEU:HG	2.38	0.43
1:A:373:THR:HA	1:A:392:TYR:CZ	2.54	0.43
1:B:155:PRO:CD	1:B:159:MET:HE3	2.48	0.43
1:B:218:ASN:O	1:B:219:SER:C	2.57	0.43
1:B:637:THR:OG1	1:B:651:ARG:CG	2.67	0.43
1:C:605:GLU:CG	1:D:524:PRO:HD3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:ILE:HG23	1:D:441:ILE:HB	2.01	0.43
1:D:694:TRP:HA	1:D:738:MET:HE2	2.01	0.43
1:E:860:TYR:OH	1:E:885:PRO:HD3	2.19	0.43
1:F:633:LYS:HE2	1:F:633:LYS:HB2	1.87	0.43
1:B:235:PRO:HA	1:B:243:TYR:O	2.19	0.42
1:B:626:THR:O	1:B:627:ARG:HB2	2.18	0.42
1:C:1055:LEU:O	1:C:1059:LEU:HD13	2.19	0.42
1:D:241:ARG:HH12	1:D:263:ASP:HB3	1.84	0.42
1:D:480:ILE:N	1:D:494:THR:HG22	2.30	0.42
1:F:53:ILE:CG2	1:F:286:LEU:HD21	2.46	0.42
1:A:994:ILE:HG22	1:A:1008:GLN:O	2.18	0.42
1:B:184:LEU:HB2	1:B:191:VAL:HB	1.99	0.42
1:B:404:LEU:HD22	1:B:429:MET:HE1	2.01	0.42
1:B:739:GLN:NE2	2:B:3141:HOH:O	2.52	0.42
1:C:936:ASP:HB2	1:C:944:SER:HB2	2.01	0.42
1:C:1031:VAL:O	1:C:1033:ILE:HD12	2.19	0.42
1:D:929:MET:HA	1:D:929:MET:HE3	2.01	0.42
1:D:992:VAL:HG11	1:D:1009:PRO:HB2	2.00	0.42
1:E:241:ARG:NH1	1:E:263:ASP:HB3	2.34	0.42
1:E:731:LEU:CD2	1:E:735:ILE:HG13	2.49	0.42
1:F:241:ARG:HH12	1:F:263:ASP:CG	2.22	0.42
1:F:731:LEU:HD22	1:F:735:ILE:HG13	2.01	0.42
1:B:319:ILE:HA	1:B:678:LEU:O	2.19	0.42
1:B:676:ARG:HA	1:B:677:PRO:HD3	1.91	0.42
1:C:156:PHE:HD1	1:C:159:MET:HE1	1.84	0.42
1:C:562:GLU:HB3	1:C:563:ALA:H	1.65	0.42
1:C:922:GLN:HE22	1:D:948:THR:N	1.98	0.42
2:C:4075:HOH:O	1:D:949:ASN:HB2	2.18	0.42
1:D:45:ASN:N	1:D:45:ASN:ND2	2.64	0.42
1:D:177:LEU:HD13	1:D:192:ILE:HD11	2.01	0.42
1:D:390:TYR:HD1	1:D:397:ALA:HB2	1.84	0.42
1:F:110:PHE:CD2	1:F:121:ILE:HG13	2.54	0.42
1:F:146:LEU:HD23	1:F:165:VAL:HG21	2.01	0.42
1:F:425:ARG:O	1:F:426:PHE:HB2	2.19	0.42
1:F:1031:VAL:HG12	1:F:1033:ILE:HD11	2.01	0.42
1:A:46:PRO:CG	1:A:286:LEU:HG	2.49	0.42
1:A:578:ILE:CD1	1:A:595:ILE:HD12	2.49	0.42
1:B:321:ILE:HB	1:B:324:LYS:HG3	2.01	0.42
1:B:562:GLU:HB3	1:B:563:ALA:H	1.59	0.42
1:C:764:ARG:HB3	1:C:855:ASP:OD1	2.19	0.42
1:C:809:ASP:HB3	1:C:814:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1031:VAL:O	1:F:1033:ILE:HD12	2.19	0.42
1:A:390:TYR:HD1	1:A:397:ALA:HB2	1.85	0.42
1:A:892:LEU:HD13	1:A:920:VAL:HG21	2.01	0.42
1:B:228:MET:CE	1:B:232:VAL:HG22	2.49	0.42
1:B:367:VAL:HG12	1:B:375:VAL:HG21	2.01	0.42
1:C:61:LEU:HB3	1:C:75:VAL:CG1	2.48	0.42
1:C:894:GLU:OE2	1:C:897:ARG:HD2	2.19	0.42
1:D:368:ARG:O	1:D:375:VAL:CG2	2.67	0.42
1:E:216:GLU:OE1	1:E:220:GLY:N	2.52	0.42
1:E:279:ASN:ND2	2:E:6071:HOH:O	2.52	0.42
1:E:389:ILE:HD11	1:E:433:LEU:HB3	2.01	0.42
1:E:913:ARG:NH2	1:E:1047:GLN:HE21	2.15	0.42
1:A:157:SER:HB2	2:A:2397:HOH:O	2.19	0.42
1:A:312:GLU:HG2	1:A:314:PRO:HD3	2.01	0.42
1:A:579:ASN:ND2	1:A:627:ARG:NH1	2.68	0.42
1:A:890:MET:O	1:A:894:GLU:HG2	2.19	0.42
1:B:167:ASN:O	1:B:170:ILE:HG12	2.20	0.42
1:B:1045:ASP:HB3	1:B:1048:ILE:HG22	2.01	0.42
1:E:897:ARG:HB2	1:F:520:LEU:HD12	2.01	0.42
1:F:936:ASP:HB2	1:F:944:SER:HB2	2.02	0.42
1:A:53:ILE:HG23	1:A:286:LEU:CD2	2.48	0.42
1:A:315:GLU:OE2	1:D:119:LYS:HD2	2.20	0.42
1:A:469:HIS:CG	1:A:470:GLY:N	2.86	0.42
1:A:676:ARG:HA	1:A:677:PRO:HD3	1.89	0.42
1:A:811:ASP:HB2	1:A:828:LYS:HE2	2.01	0.42
1:C:258:ASP:C	1:C:260:ASP:H	2.21	0.42
1:C:596:LEU:N	1:C:596:LEU:HD22	2.35	0.42
1:C:926:GLU:CG	1:D:926:GLU:HG2	2.50	0.42
1:E:926:GLU:CG	1:F:926:GLU:HG2	2.50	0.42
1:B:53:ILE:HG12	1:B:286:LEU:HD22	2.01	0.42
1:C:295:ILE:HG13	1:C:306:ILE:HD11	2.02	0.42
1:C:530:ASN:ND2	1:C:531:PHE:N	2.66	0.42
1:C:887:MET:HB3	1:C:966:ASP:OD2	2.20	0.42
1:C:1052:ILE:O	1:C:1056:ILE:HG13	2.19	0.42
1:D:153:MET:HG3	1:D:859:ARG:NH1	2.35	0.42
1:D:357:LYS:HB2	1:D:676:ARG:HH12	1.84	0.42
1:E:362:LEU:HD23	1:E:362:LEU:HA	1.84	0.42
1:E:926:GLU:HG2	1:F:926:GLU:CG	2.49	0.42
1:F:110:PHE:CE2	1:F:121:ILE:HG13	2.55	0.42
1:F:230:THR:HG21	1:F:248:ILE:HA	2.02	0.42
1:F:362:LEU:HD23	1:F:362:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:462:ALA:HA	1:F:481:HIS:O	2.20	0.42
1:A:501:TYR:N	1:A:501:TYR:CD2	2.87	0.42
1:A:635:ASN:HB3	1:A:653:ASP:OD1	2.19	0.42
1:B:153:MET:HG3	1:B:859:ARG:NH1	2.34	0.42
1:B:217:VAL:HG23	1:B:218:ASN:N	2.35	0.42
1:B:373:THR:HA	1:B:392:TYR:CZ	2.54	0.42
1:C:153:MET:HG3	1:C:859:ARG:CZ	2.50	0.42
1:C:362:LEU:HD23	1:C:362:LEU:HA	1.85	0.42
1:C:367:VAL:CG1	1:C:375:VAL:HG21	2.50	0.42
1:C:499:HIS:HD2	2:C:4176:HOH:O	2.02	0.42
1:D:286:LEU:HD13	1:D:295:ILE:HG12	2.00	0.42
1:D:494:THR:CG2	1:D:500:ASP:OD1	2.65	0.42
1:F:494:THR:HG21	1:F:500:ASP:OD1	2.20	0.42
1:F:929:MET:HA	1:F:929:MET:CE	2.49	0.42
1:A:189:ARG:HB2	1:A:216:GLU:HB3	2.01	0.42
1:B:807:ILE:HG12	1:B:837:LEU:CD2	2.50	0.42
1:C:350:VAL:HG11	1:C:669:ARG:NH1	2.35	0.42
1:E:206:ARG:N	1:E:1024:ASN:HD21	2.16	0.42
1:F:345:ALA:HB2	1:F:364:ILE:HG21	2.01	0.42
1:F:436:GLY:O	1:F:438:PRO:HD3	2.20	0.42
1:F:469:HIS:HD1	1:F:473:ASP:CG	2.23	0.42
1:A:279:ASN:HD22	1:A:279:ASN:HA	1.78	0.41
1:B:641:LEU:HD22	1:B:645:ARG:HA	2.02	0.41
1:B:989:GLY:HA2	1:B:1026:GLY:HA2	2.03	0.41
1:B:1031:VAL:HG12	1:B:1033:ILE:HD11	2.01	0.41
1:C:117:GLU:HA	1:F:313:SER:HB3	2.01	0.41
1:C:423:ASN:ND2	1:C:427:GLU:H	2.18	0.41
1:C:977:LEU:HB2	1:C:979:LEU:CD1	2.49	0.41
1:D:216:GLU:OE1	1:D:219:SER:HA	2.20	0.41
1:D:390:TYR:CD1	1:D:397:ALA:HB2	2.55	0.41
1:D:589:ILE:HB	1:D:596:LEU:HB2	2.02	0.41
1:E:423:ASN:ND2	1:E:425:ARG:HB2	2.35	0.41
1:F:322:PRO:HG2	1:F:674:ASP:OD1	2.19	0.41
1:A:428:ILE:HG23	1:A:441:ILE:HB	2.02	0.41
1:B:119:LYS:HZ1	1:B:823:ARG:HH22	1.66	0.41
1:B:278:LEU:HD23	1:B:287:PHE:HB3	2.02	0.41
1:B:469:HIS:CG	1:B:470:GLY:N	2.88	0.41
1:C:402:GLU:HG3	1:C:438:PRO:HD3	2.02	0.41
1:C:446:GLU:OE1	1:C:468:LYS:HE2	2.19	0.41
1:C:616:LYS:HE2	1:C:653:ASP:CB	2.49	0.41
1:F:203:LYS:HD3	1:F:740:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:811:ASP:HB2	1:F:828:LYS:HE2	2.02	0.41
1:A:228:MET:HE3	1:A:232:VAL:HG21	2.02	0.41
1:B:425:ARG:HB3	1:B:427:GLU:HG3	2.02	0.41
1:B:731:LEU:HD22	1:B:735:ILE:HG13	2.02	0.41
1:B:871:VAL:HG22	1:B:1052:ILE:HD11	2.01	0.41
1:C:241:ARG:HH12	1:C:263:ASP:HB3	1.84	0.41
1:C:875:SER:HB2	1:C:879:ILE:HG13	2.02	0.41
1:F:253:GLN:NE2	1:F:253:GLN:HA	2.35	0.41
1:A:110:PHE:CD2	1:A:121:ILE:HG13	2.54	0.41
1:B:156:PHE:H	1:B:159:MET:CE	2.34	0.41
1:B:401:GLU:OE2	1:B:401:GLU:N	2.47	0.41
1:C:82:ASN:HD21	1:C:96:ARG:HH21	1.67	0.41
1:D:155:PRO:HB3	1:D:860:TYR:HA	2.02	0.41
1:D:218:ASN:O	1:D:221:ALA:N	2.53	0.41
1:D:241:ARG:NH1	1:D:263:ASP:HB3	2.35	0.41
1:D:368:ARG:O	1:D:375:VAL:HG23	2.21	0.41
1:D:676:ARG:NH2	2:D:5370:HOH:O	2.53	0.41
1:E:247:ASP:HA	1:E:251:PHE:O	2.20	0.41
1:E:253:GLN:HB2	1:E:255:TYR:CE1	2.55	0.41
1:F:807:ILE:HG12	1:F:837:LEU:CD2	2.50	0.41
1:F:905:TYR:HB2	2:F:7042:HOH:O	2.18	0.41
1:B:78:LEU:HD11	1:B:118:ILE:HD11	2.02	0.41
1:C:184:LEU:HB2	1:C:191:VAL:HB	2.01	0.41
1:D:735:ILE:O	1:D:739:GLN:HG3	2.20	0.41
1:D:881:TYR:O	1:D:902:GLU:HG3	2.20	0.41
1:D:947:PRO:HD2	1:D:950:SER:HB3	2.02	0.41
1:E:642:SER:HB3	1:E:647:THR:H	1.84	0.41
1:F:89:ASP:OD1	1:F:91:ARG:HG3	2.21	0.41
1:F:992:VAL:HG11	1:F:1009:PRO:HB2	2.02	0.41
1:A:194:ARG:O	1:A:211:GLY:HA2	2.21	0.41
1:A:524:PRO:HD3	1:B:605:GLU:HG3	2.01	0.41
1:B:46:PRO:CG	1:B:286:LEU:HG	2.50	0.41
1:B:618:VAL:CG2	1:B:631:GLU:HG3	2.51	0.41
1:C:43:LEU:HD13	1:C:308:ILE:HD12	2.03	0.41
1:C:319:ILE:HA	1:C:678:LEU:O	2.20	0.41
1:D:228:MET:HE1	1:D:244:PHE:CE1	2.55	0.41
1:F:767:CYS:HA	1:F:780:LYS:O	2.20	0.41
1:A:295:ILE:HG13	1:A:306:ILE:HD11	2.02	0.41
1:A:1031:VAL:O	1:A:1033:ILE:HD12	2.21	0.41
1:B:74:ILE:HG13	1:B:75:VAL:HG12	2.02	0.41
1:B:228:MET:CE	1:B:244:PHE:CE1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ASP:CG	1:B:369:ARG:HE	2.24	0.41
1:B:423:ASN:ND2	1:B:425:ARG:HB2	2.36	0.41
1:B:1055:LEU:O	1:B:1059:LEU:HD13	2.21	0.41
1:D:423:ASN:HD22	1:D:423:ASN:C	2.24	0.41
1:D:703:ASN:C	1:D:703:ASN:ND2	2.71	0.41
1:E:74:ILE:HG13	1:E:75:VAL:HG12	2.03	0.41
1:E:228:MET:HE2	1:E:244:PHE:CZ	2.56	0.41
1:F:155:PRO:HB3	1:F:860:TYR:HA	2.03	0.41
1:F:912:VAL:HG22	1:F:958:ILE:O	2.21	0.41
1:C:118:ILE:HG22	1:F:314:PRO:HA	2.02	0.41
1:C:350:VAL:CG2	1:C:669:ARG:NH1	2.83	0.41
1:E:722:VAL:N	1:E:723:PRO:HD2	2.36	0.41
1:E:791:GLU:CD	1:E:861:ARG:HE	2.24	0.41
1:F:119:LYS:NZ	1:F:823:ARG:HH22	2.19	0.41
1:F:170:ILE:HD13	1:F:820:ASN:HB2	2.02	0.41
1:A:85:ARG:HD3	2:A:2104:HOH:O	2.21	0.41
1:A:156:PHE:CD1	1:A:159:MET:CE	3.04	0.41
1:A:591:LEU:HD12	1:A:596:LEU:HD23	2.02	0.41
1:A:802:PRO:O	1:A:805:TYR:HB2	2.21	0.41
1:A:886:ASP:O	1:A:891:GLY:HA3	2.21	0.41
1:B:119:LYS:NZ	1:B:823:ARG:NH2	2.69	0.41
1:B:591:LEU:HD11	1:B:662:LEU:HD21	2.02	0.41
1:B:624:VAL:HG23	1:B:625:LYS:N	2.36	0.41
1:B:694:TRP:HA	1:B:738:MET:CE	2.51	0.41
1:B:965:SER:N	1:B:968:ASP:OD2	2.51	0.41
1:C:96:ARG:NH2	1:C:133:MET:HB3	2.35	0.41
1:C:253:GLN:HB2	1:C:255:TYR:HE1	1.86	0.41
1:C:480:ILE:N	1:C:494:THR:HG22	2.28	0.41
1:C:714:ILE:HG21	1:C:741:GLU:HG3	2.03	0.41
1:D:155:PRO:HD2	1:D:159:MET:HE3	2.02	0.41
1:D:190:ARG:NH2	1:D:190:ARG:CG	2.83	0.41
1:D:268:THR:HG22	1:D:303:ILE:CD1	2.45	0.41
1:D:599:SER:HB3	1:D:618:VAL:HG13	2.03	0.41
1:D:895:PHE:CE2	1:D:924:ILE:HG23	2.56	0.41
1:E:136:ASP:OD2	1:E:137:VAL:N	2.44	0.41
1:E:236:VAL:HG23	1:E:243:TYR:HB2	2.03	0.41
1:E:565:GLU:CG	1:E:566:TYR:N	2.83	0.41
1:E:580:VAL:HG22	1:E:622:TYR:CD2	2.56	0.41
1:E:1016:ARG:O	1:E:1017:ASP:CB	2.69	0.41
1:F:46:PRO:HB2	1:F:286:LEU:HD23	2.02	0.41
1:F:160:THR:O	1:F:179:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:ILE:O	1:F:256:SER:HA	2.21	0.41
1:F:383:GLU:OE2	1:F:383:GLU:HA	2.20	0.41
1:F:546:PRO:CG	1:F:567:ASP:HB3	2.51	0.41
1:F:628:LYS:HE2	1:F:628:LYS:HB3	1.88	0.41
1:F:706:VAL:HG12	1:F:710:ILE:HD11	2.02	0.41
1:F:708:LYS:O	1:F:712:GLU:HG3	2.21	0.41
1:A:72:ARG:HG3	1:D:72:ARG:HG3	2.03	0.41
1:A:130:GLY:HA3	2:A:2163:HOH:O	2.20	0.41
1:B:123:TYR:OH	1:B:823:ARG:HD3	2.21	0.41
1:B:346:PHE:C	1:B:347:ILE:HD12	2.42	0.41
1:B:628:LYS:HE2	1:B:628:LYS:HB3	1.94	0.41
1:B:892:LEU:HD12	1:B:892:LEU:HA	1.96	0.41
1:C:216:GLU:OE1	1:C:219:SER:HA	2.21	0.41
1:C:253:GLN:NE2	1:C:268:THR:OG1	2.49	0.41
1:C:393:ARG:HH12	1:E:557:ARG:HD2	1.86	0.41
1:C:887:MET:O	1:C:920:VAL:HG22	2.21	0.41
1:F:591:LEU:HD11	1:F:662:LEU:HD21	2.03	0.41
1:F:739:GLN:NE2	2:F:7141:HOH:O	2.53	0.41
1:A:110:PHE:CE2	1:A:146:LEU:HD22	2.55	0.40
1:A:286:LEU:HD11	1:A:293:ILE:HG22	2.03	0.40
1:A:308:ILE:HG22	1:A:311:LEU:HD11	2.02	0.40
1:A:466:PRO:HB3	2:A:2183:HOH:O	2.20	0.40
1:A:618:VAL:HG23	1:A:633:LYS:O	2.20	0.40
1:B:297:ASN:O	1:B:301:GLU:N	2.46	0.40
1:B:337:ILE:CG2	1:B:338:ALA:N	2.84	0.40
1:B:498:SER:OG	1:B:499:HIS:N	2.54	0.40
1:C:183:ILE:O	1:C:183:ILE:HG23	2.21	0.40
1:C:194:ARG:O	1:C:211:GLY:HA2	2.22	0.40
1:C:210:ARG:HH21	1:C:210:ARG:HG2	1.87	0.40
1:C:499:HIS:HE1	2:C:4239:HOH:O	2.04	0.40
1:C:735:ILE:O	1:C:738:MET:HG3	2.21	0.40
1:C:947:PRO:HG3	2:C:4038:HOH:O	2.20	0.40
1:D:134:PHE:O	1:D:135:THR:HB	2.21	0.40
1:D:403:ASN:HD22	1:D:404:LEU:N	2.19	0.40
1:D:499:HIS:HD2	2:D:5176:HOH:O	2.04	0.40
1:E:731:LEU:HD22	1:E:735:ILE:CD1	2.52	0.40
1:F:373:THR:HG21	1:F:393:ARG:HD2	2.03	0.40
1:F:956:ILE:HG22	1:F:1055:LEU:HD11	2.01	0.40
1:B:156:PHE:HD1	1:B:159:MET:HE1	1.84	0.40
1:B:332:LEU:HD11	1:B:338:ALA:HB2	2.03	0.40
1:B:690:TYR:OH	1:B:718:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LEU:O	1:C:176:ASN:HB2	2.21	0.40
1:C:300:THR:O	1:C:301:GLU:HB3	2.21	0.40
1:D:88:PRO:HG3	1:D:144:GLY:HA2	2.01	0.40
1:E:338:ALA:HA	1:E:346:PHE:O	2.21	0.40
1:E:872:HIS:CE1	1:E:902:GLU:OE1	2.72	0.40
1:F:155:PRO:HD2	1:F:159:MET:HE3	2.04	0.40
1:F:929:MET:HA	1:F:929:MET:HE3	2.02	0.40
1:A:350:VAL:CG2	1:A:669:ARG:NH1	2.83	0.40
1:A:589:ILE:HB	1:A:596:LEU:HB2	2.04	0.40
1:B:559:MET:HG2	1:D:356:LEU:HD11	2.02	0.40
1:B:811:ASP:HB2	1:B:828:LYS:HE2	2.03	0.40
1:B:860:TYR:OH	1:B:885:PRO:HD3	2.21	0.40
1:C:141:ASP:HB2	1:C:142:PRO:CD	2.51	0.40
1:C:423:ASN:ND2	1:C:425:ARG:HB2	2.36	0.40
1:C:633:LYS:HE2	1:C:633:LYS:HB2	1.88	0.40
1:E:892:LEU:HD13	1:E:920:VAL:HG21	2.03	0.40
1:F:279:ASN:ND2	2:F:7071:HOH:O	2.54	0.40
1:A:235:PRO:HA	1:A:243:TYR:O	2.20	0.40
1:A:319:ILE:HG23	1:A:677:PRO:CB	2.51	0.40
1:A:387:LEU:HD12	1:A:400:PHE:CE1	2.56	0.40
1:A:731:LEU:HD22	1:A:735:ILE:HG13	2.04	0.40
1:B:123:TYR:HB3	1:B:826:SER:OG	2.22	0.40
1:E:183:ILE:HA	1:E:191:VAL:O	2.21	0.40
1:E:446:GLU:CD	1:E:468:LYS:HG3	2.42	0.40
1:E:628:LYS:HE3	2:E:6366:HOH:O	2.22	0.40
1:F:640:ARG:HG2	1:F:640:ARG:HH21	1.86	0.40
1:F:884:ILE:HA	1:F:885:PRO:HD2	1.83	0.40
1:A:270:PHE:CE2	1:A:289:LYS:HE2	2.56	0.40
1:A:489:LYS:HE2	1:A:491:PHE:CZ	2.53	0.40
1:B:342:ARG:NE	1:B:685:GLU:OE1	2.51	0.40
1:B:530:ASN:ND2	1:B:531:PHE:H	2.20	0.40
1:C:156:PHE:H	1:C:159:MET:CE	2.35	0.40
1:C:578:ILE:O	1:C:580:VAL:N	2.50	0.40
1:C:589:ILE:HG21	1:C:641:LEU:CD1	2.52	0.40
1:E:141:ASP:HB2	1:E:142:PRO:HD2	2.04	0.40
1:E:619:LEU:HD13	1:E:639:LEU:HD13	2.04	0.40
1:F:703:ASN:C	1:F:703:ASN:HD22	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1045 (98%)	979 (96%)	38 (4%)	4 (0%)	34	30
1	B	1021/1045 (98%)	977 (96%)	41 (4%)	3 (0%)	41	37
1	C	1021/1045 (98%)	961 (94%)	53 (5%)	7 (1%)	22	16
1	D	1021/1045 (98%)	979 (96%)	38 (4%)	4 (0%)	34	30
1	E	1021/1045 (98%)	975 (96%)	43 (4%)	3 (0%)	41	37
1	F	1021/1045 (98%)	971 (95%)	44 (4%)	6 (1%)	25	19
All	All	6126/6270 (98%)	5842 (95%)	257 (4%)	27 (0%)	34	30

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ASP
1	B	328	ASP
1	C	219	SER
1	C	579	ASN
1	D	219	SER
1	E	219	SER
1	F	219	SER
1	F	579	ASN
1	A	562	GLU
1	B	562	GLU
1	B	579	ASN
1	C	562	GLU
1	E	562	GLU
1	E	579	ASN
1	F	562	GLU
1	F	563	ALA
1	D	562	GLU
1	A	219	SER
1	C	328	ASP
1	D	563	ALA

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Mol	Chain	Res	Type
1	D	579	ASN
1	F	259	LEU
1	A	579	ASN
1	C	563	ALA
1	C	665	PRO
1	C	45	ASN
1	F	682	ILE

5.3.2 Protein sidechains [i](#)

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	883/904 (98%)	857 (97%)	26 (3%)	42	43
1	B	883/904 (98%)	853 (97%)	30 (3%)	37	36
1	C	883/904 (98%)	860 (97%)	23 (3%)	46	48
1	D	883/904 (98%)	856 (97%)	27 (3%)	40	40
1	E	883/904 (98%)	857 (97%)	26 (3%)	42	43
1	F	883/904 (98%)	857 (97%)	26 (3%)	42	43
All	All	5298/5424 (98%)	5140 (97%)	158 (3%)	41	41

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	46	PRO
1	A	61	LEU
1	A	104	ASN
1	A	190	ARG
1	A	279	ASN
1	A	311	LEU
1	A	313	SER
1	A	363	ARG
1	A	375	VAL
1	A	403	ASN

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Mol	Chain	Res	Type
1	A	423	ASN
1	A	469	HIS
1	A	562	GLU
1	A	578	ILE
1	A	641	LEU
1	A	678	LEU
1	A	687	LEU
1	A	703	ASN
1	A	719	ARG
1	A	731	LEU
1	A	738	MET
1	A	929	MET
1	A	965	SER
1	A	1024	ASN
1	A	1035	TYR
1	B	44	LEU
1	B	61	LEU
1	B	75	VAL
1	B	104	ASN
1	B	114	GLU
1	B	153	MET
1	B	190	ARG
1	B	279	ASN
1	B	311	LEU
1	B	313	SER
1	B	330	SER
1	B	363	ARG
1	B	403	ASN
1	B	423	ASN
1	B	469	HIS
1	B	481	HIS
1	B	557	ARG
1	B	562	GLU
1	B	578	ILE
1	B	641	LEU
1	B	678	LEU
1	B	687	LEU
1	B	703	ASN
1	B	717	LYS
1	B	719	ARG
1	B	731	LEU
1	B	738	MET

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Mol	Chain	Res	Type
1	B	892	LEU
1	B	1024	ASN
1	B	1035	TYR
1	C	61	LEU
1	C	75	VAL
1	C	82	ASN
1	C	104	ASN
1	C	279	ASN
1	C	353	THR
1	C	363	ARG
1	C	403	ASN
1	C	423	ASN
1	C	469	HIS
1	C	481	HIS
1	C	557	ARG
1	C	562	GLU
1	C	578	ILE
1	C	641	LEU
1	C	687	LEU
1	C	703	ASN
1	C	719	ARG
1	C	731	LEU
1	C	738	MET
1	C	892	LEU
1	C	1024	ASN
1	C	1035	TYR
1	D	61	LEU
1	D	75	VAL
1	D	82	ASN
1	D	104	ASN
1	D	114	GLU
1	D	190	ARG
1	D	218	ASN
1	D	279	ASN
1	D	311	LEU
1	D	363	ARG
1	D	403	ASN
1	D	423	ASN
1	D	469	HIS
1	D	532	SER
1	D	557	ARG
1	D	562	GLU

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Mol	Chain	Res	Type
1	D	578	ILE
1	D	641	LEU
1	D	687	LEU
1	D	703	ASN
1	D	719	ARG
1	D	731	LEU
1	D	738	MET
1	D	809	ASP
1	D	892	LEU
1	D	1024	ASN
1	D	1035	TYR
1	E	44	LEU
1	E	61	LEU
1	E	75	VAL
1	E	82	ASN
1	E	104	ASN
1	E	114	GLU
1	E	190	ARG
1	E	209	THR
1	E	218	ASN
1	E	311	LEU
1	E	363	ARG
1	E	403	ASN
1	E	423	ASN
1	E	469	HIS
1	E	557	ARG
1	E	562	GLU
1	E	578	ILE
1	E	641	LEU
1	E	703	ASN
1	E	719	ARG
1	E	731	LEU
1	E	738	MET
1	E	809	ASP
1	E	892	LEU
1	E	1024	ASN
1	E	1035	TYR
1	F	44	LEU
1	F	46	PRO
1	F	61	LEU
1	F	75	VAL
1	F	190	ARG

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Mol	Chain	Res	Type
1	F	209	THR
1	F	279	ASN
1	F	363	ARG
1	F	403	ASN
1	F	423	ASN
1	F	469	HIS
1	F	481	HIS
1	F	557	ARG
1	F	562	GLU
1	F	578	ILE
1	F	641	LEU
1	F	687	LEU
1	F	703	ASN
1	F	719	ARG
1	F	731	LEU
1	F	738	MET
1	F	892	LEU
1	F	929	MET
1	F	1008	GLN
1	F	1024	ASN
1	F	1035	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (193) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	64	HIS
1	A	82	ASN
1	A	104	ASN
1	A	176	ASN
1	A	253	GLN
1	A	267	HIS
1	A	279	ASN
1	A	403	ASN
1	A	415	ASN
1	A	423	ASN
1	A	481	HIS
1	A	497	ASN
1	A	499	HIS
1	A	511	ASN
1	A	530	ASN
1	A	579	ASN

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Mol	Chain	Res	Type
1	A	611	GLN
1	A	635	ASN
1	A	703	ASN
1	A	733	ASN
1	A	739	GLN
1	A	867	ASN
1	A	872	HIS
1	A	922	GLN
1	A	930	ASN
1	A	949	ASN
1	A	1008	GLN
1	A	1024	ASN
1	A	1038	HIS
1	A	1047	GLN
1	B	45	ASN
1	B	64	HIS
1	B	82	ASN
1	B	104	ASN
1	B	253	GLN
1	B	267	HIS
1	B	279	ASN
1	B	403	ASN
1	B	415	ASN
1	B	423	ASN
1	B	481	HIS
1	B	497	ASN
1	B	499	HIS
1	B	511	ASN
1	B	530	ASN
1	B	579	ASN
1	B	611	GLN
1	B	635	ASN
1	B	703	ASN
1	B	733	ASN
1	B	739	GLN
1	B	867	ASN
1	B	872	HIS
1	B	922	GLN
1	B	930	ASN
1	B	949	ASN
1	B	1008	GLN
1	B	1024	ASN

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Mol	Chain	Res	Type
1	B	1038	HIS
1	B	1047	GLN
1	C	45	ASN
1	C	49	HIS
1	C	64	HIS
1	C	82	ASN
1	C	104	ASN
1	C	195	ASN
1	C	253	GLN
1	C	267	HIS
1	C	279	ASN
1	C	403	ASN
1	C	423	ASN
1	C	497	ASN
1	C	499	HIS
1	C	511	ASN
1	C	530	ASN
1	C	579	ASN
1	C	611	GLN
1	C	635	ASN
1	C	703	ASN
1	C	720	ASN
1	C	733	ASN
1	C	739	GLN
1	C	867	ASN
1	C	872	HIS
1	C	922	GLN
1	C	930	ASN
1	C	949	ASN
1	C	1008	GLN
1	C	1024	ASN
1	C	1038	HIS
1	C	1047	GLN
1	D	45	ASN
1	D	49	HIS
1	D	64	HIS
1	D	82	ASN
1	D	104	ASN
1	D	253	GLN
1	D	267	HIS
1	D	279	ASN
1	D	403	ASN

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Mol	Chain	Res	Type
1	D	415	ASN
1	D	423	ASN
1	D	481	HIS
1	D	497	ASN
1	D	499	HIS
1	D	511	ASN
1	D	530	ASN
1	D	569	ASN
1	D	611	GLN
1	D	635	ASN
1	D	703	ASN
1	D	720	ASN
1	D	733	ASN
1	D	739	GLN
1	D	867	ASN
1	D	872	HIS
1	D	922	GLN
1	D	930	ASN
1	D	937	ASN
1	D	949	ASN
1	D	1008	GLN
1	D	1024	ASN
1	D	1038	HIS
1	D	1047	GLN
1	E	45	ASN
1	E	49	HIS
1	E	64	HIS
1	E	82	ASN
1	E	104	ASN
1	E	253	GLN
1	E	267	HIS
1	E	279	ASN
1	E	403	ASN
1	E	415	ASN
1	E	423	ASN
1	E	481	HIS
1	E	497	ASN
1	E	499	HIS
1	E	511	ASN
1	E	530	ASN
1	E	569	ASN
1	E	611	GLN

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Mol	Chain	Res	Type
1	E	635	ASN
1	E	703	ASN
1	E	720	ASN
1	E	733	ASN
1	E	739	GLN
1	E	867	ASN
1	E	872	HIS
1	E	901	ASN
1	E	922	GLN
1	E	930	ASN
1	E	949	ASN
1	E	1008	GLN
1	E	1024	ASN
1	E	1038	HIS
1	E	1047	GLN
1	F	45	ASN
1	F	64	HIS
1	F	82	ASN
1	F	104	ASN
1	F	145	ASN
1	F	176	ASN
1	F	253	GLN
1	F	267	HIS
1	F	279	ASN
1	F	403	ASN
1	F	415	ASN
1	F	423	ASN
1	F	481	HIS
1	F	497	ASN
1	F	499	HIS
1	F	511	ASN
1	F	530	ASN
1	F	569	ASN
1	F	579	ASN
1	F	611	GLN
1	F	635	ASN
1	F	703	ASN
1	F	720	ASN
1	F	733	ASN
1	F	739	GLN
1	F	867	ASN
1	F	872	HIS

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Mol	Chain	Res	Type
1	F	901	ASN
1	F	922	GLN
1	F	930	ASN
1	F	949	ASN
1	F	1008	GLN
1	F	1024	ASN
1	F	1038	HIS
1	F	1047	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 monosaccharides 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	1022/1045 (97%)	0.23	31 (3%) 50 49	14, 26, 43, 56	19 (1%)
1	B	1022/1045 (97%)	0.22	28 (2%) 54 53	16, 26, 43, 55	19 (1%)
1	C	1022/1045 (97%)	0.68	117 (11%) 5 4	20, 33, 46, 56	19 (1%)
1	D	1022/1045 (97%)	0.27	45 (4%) 34 33	18, 28, 45, 54	19 (1%)
1	E	1022/1045 (97%)	0.24	33 (3%) 47 46	17, 28, 45, 55	19 (1%)
1	F	1022/1045 (97%)	0.63	106 (10%) 6 5	21, 32, 46, 55	19 (1%)
All	All	6132/6270 (97%)	0.38	360 (5%) 22 21	14, 30, 45, 56	114 (1%)

All (360) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	SER	9.0
1	F	219	SER	8.9
1	A	841	GLY	8.7
1	F	220	GLY	8.1
1	D	219	SER	7.9
1	E	219	SER	7.7
1	C	841	GLY	7.5
1	E	220	GLY	7.3
1	F	563	ALA	7.0
1	C	220	GLY	6.8
1	C	218	ASN	6.5
1	C	188	GLY	6.3
1	E	218	ASN	6.3
1	D	220	GLY	6.2
1	C	238	VAL	5.8
1	C	842	GLY	5.6
1	C	563	ALA	5.5
1	F	839	GLY	5.4
1	F	840	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	299	ASP	5.2
1	C	217	VAL	5.2
1	C	300	THR	5.0
1	B	563	ALA	5.0
1	F	69	GLY	4.9
1	F	706	VAL	4.9
1	D	841	GLY	4.9
1	C	116	GLY	4.8
1	F	188	GLY	4.8
1	F	67	LYS	4.8
1	D	842	GLY	4.8
1	C	299	ASP	4.8
1	C	840	LYS	4.7
1	C	774	ASP	4.7
1	C	706	VAL	4.7
1	B	218	ASN	4.7
1	F	843	ASP	4.6
1	D	563	ALA	4.6
1	C	562	GLU	4.5
1	D	435	THR	4.5
1	C	66	LEU	4.5
1	F	842	GLY	4.4
1	C	843	ASP	4.4
1	D	218	ASN	4.3
1	C	67	LYS	4.3
1	D	840	LYS	4.3
1	C	69	GLY	4.3
1	B	841	GLY	4.1
1	C	221	ALA	4.1
1	C	142	PRO	4.1
1	D	436	GLY	4.1
1	D	469	HIS	4.1
1	C	806	LEU	4.1
1	C	239	GLY	4.1
1	F	774	ASP	4.1
1	F	434	GLU	4.0
1	F	771	LEU	4.0
1	F	218	ASN	4.0
1	C	114	GLU	4.0
1	F	262	LYS	4.0
1	C	817	ALA	4.0
1	D	706	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	305	LYS	3.9
1	F	561	SER	3.9
1	C	752	GLY	3.9
1	F	401	GLU	3.8
1	F	217	VAL	3.8
1	C	839	GLY	3.8
1	F	393	ARG	3.8
1	F	238	VAL	3.8
1	F	806	LEU	3.8
1	A	563	ALA	3.7
1	C	707	ALA	3.7
1	D	434	GLU	3.7
1	C	318	ILE	3.6
1	C	68	SER	3.6
1	F	187	ASP	3.6
1	F	435	THR	3.6
1	C	1043	GLY	3.5
1	F	300	THR	3.5
1	F	841	GLY	3.5
1	E	469	HIS	3.5
1	B	434	GLU	3.5
1	F	705	ALA	3.5
1	E	842	GLY	3.5
1	D	843	ASP	3.4
1	F	488	ARG	3.4
1	C	654	ASP	3.4
1	D	299	ASP	3.4
1	D	667	ASP	3.4
1	F	612	GLY	3.4
1	C	187	ASP	3.4
1	D	1019	GLY	3.4
1	C	777	VAL	3.4
1	F	70	SER	3.4
1	B	39	MET	3.3
1	F	65	ASP	3.3
1	F	704	GLU	3.3
1	C	237	ILE	3.3
1	A	434	GLU	3.3
1	C	51	ASP	3.3
1	F	260	ASP	3.2
1	F	66	LEU	3.2
1	C	144	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	397	ALA	3.2
1	F	297	ASN	3.2
1	C	561	SER	3.2
1	C	667	ASP	3.2
1	E	841	GLY	3.2
1	C	65	ASP	3.2
1	D	286	LEU	3.2
1	B	488	ARG	3.1
1	A	839	GLY	3.1
1	F	215	ILE	3.1
1	F	722	VAL	3.1
1	F	307	GLU	3.1
1	C	271	THR	3.1
1	D	653	ASP	3.1
1	E	840	LYS	3.1
1	C	401	GLU	3.1
1	F	258	ASP	3.0
1	C	844	LYS	3.0
1	E	91	ARG	3.0
1	B	628	LYS	3.0
1	F	114	GLU	3.0
1	E	299	ASP	3.0
1	A	437	LYS	3.0
1	E	562	GLU	3.0
1	F	91	ARG	3.0
1	F	221	ALA	3.0
1	F	716	GLU	3.0
1	B	435	THR	3.0
1	C	91	ARG	3.0
1	F	562	GLU	3.0
1	C	303	ILE	2.9
1	B	612	GLY	2.9
1	F	272	ASP	2.9
1	E	563	ALA	2.9
1	F	51	ASP	2.9
1	F	362	LEU	2.9
1	C	168	ASP	2.9
1	F	1043	GLY	2.9
1	B	923	LEU	2.9
1	D	613	ALA	2.9
1	F	189	ARG	2.9
1	D	716	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	435	THR	2.8
1	D	91	ARG	2.8
1	C	1038	HIS	2.8
1	F	773	GLY	2.8
1	C	202	TRP	2.8
1	C	1042	SER	2.8
1	F	68	SER	2.8
1	D	839	GLY	2.8
1	C	286	LEU	2.8
1	F	186	ALA	2.8
1	E	434	GLU	2.8
1	C	297	ASN	2.8
1	D	1059	LEU	2.8
1	C	434	GLU	2.8
1	B	469	HIS	2.8
1	F	415	ASN	2.8
1	C	845	ARG	2.8
1	A	494	THR	2.7
1	C	488	ARG	2.7
1	E	1017	ASP	2.7
1	A	840	LYS	2.7
1	C	439	THR	2.7
1	F	303	ILE	2.7
1	A	67	LYS	2.7
1	A	199	LEU	2.7
1	C	705	ALA	2.7
1	F	817	ALA	2.7
1	C	722	VAL	2.7
1	C	653	ASP	2.7
1	A	469	HIS	2.7
1	C	469	HIS	2.7
1	C	50	GLY	2.7
1	F	667	ASP	2.7
1	C	487	GLY	2.7
1	F	436	GLY	2.7
1	A	562	GLU	2.7
1	D	705	ALA	2.7
1	F	50	GLY	2.7
1	B	928	LEU	2.7
1	F	775	HIS	2.6
1	C	262	LYS	2.6
1	F	469	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	218	ASN	2.6
1	D	114	GLU	2.6
1	A	39	MET	2.6
1	C	393	ARG	2.6
1	F	239	GLY	2.6
1	A	488	ARG	2.6
1	C	435	THR	2.6
1	E	592	GLU	2.6
1	D	437	LYS	2.6
1	B	924	ILE	2.6
1	D	239	GLY	2.6
1	E	436	GLY	2.6
1	D	1017	ASP	2.5
1	E	706	VAL	2.5
1	E	114	GLU	2.5
1	F	628	LYS	2.5
1	C	1041	LEU	2.5
1	D	562	GLU	2.5
1	F	1059	LEU	2.5
1	D	612	GLY	2.5
1	F	844	LYS	2.5
1	C	803	THR	2.5
1	D	557	ARG	2.5
1	E	665	PRO	2.5
1	F	142	PRO	2.5
1	C	812	GLY	2.5
1	B	1017	ASP	2.5
1	C	258	ASP	2.5
1	B	562	GLU	2.5
1	C	243	TYR	2.5
1	F	185	PHE	2.5
1	C	613	ALA	2.5
1	A	1017	ASP	2.5
1	C	612	GLY	2.5
1	C	185	PHE	2.5
1	C	665	PRO	2.4
1	D	560	THR	2.4
1	C	663	GLU	2.4
1	A	44	LEU	2.4
1	C	415	ASN	2.4
1	C	716	GLU	2.4
1	C	724	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	653	ASP	2.4
1	F	170	ILE	2.4
1	C	494	THR	2.4
1	C	683	HIS	2.4
1	A	928	LEU	2.4
1	C	70	SER	2.4
1	C	100	GLY	2.4
1	B	167	ASN	2.4
1	D	665	PRO	2.4
1	C	838	SER	2.4
1	A	842	GLY	2.4
1	F	308	ILE	2.4
1	B	557	ARG	2.4
1	C	436	GLY	2.4
1	F	494	THR	2.4
1	D	905	TYR	2.4
1	F	756	ASP	2.4
1	B	286	LEU	2.3
1	D	199	LEU	2.3
1	F	270	PHE	2.3
1	F	144	GLY	2.3
1	F	609	TYR	2.3
1	B	842	GLY	2.3
1	C	145	ASN	2.3
1	C	64	HIS	2.3
1	C	304	GLU	2.3
1	F	282	GLY	2.3
1	C	305	LYS	2.3
1	B	437	LYS	2.3
1	B	705	ALA	2.3
1	A	612	GLY	2.3
1	E	397	ALA	2.3
1	E	401	GLU	2.3
1	F	613	ALA	2.3
1	E	627	ARG	2.3
1	B	494	THR	2.2
1	C	445	ARG	2.2
1	E	612	GLY	2.2
1	A	286	LEU	2.2
1	C	771	LEU	2.2
1	F	374	LYS	2.2
1	F	625	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	237	ILE	2.2
1	F	293	ILE	2.2
1	F	240	HIS	2.2
1	C	236	VAL	2.2
1	C	758	ASP	2.2
1	C	704	GLU	2.2
1	A	627	ARG	2.2
1	C	39	MET	2.2
1	C	628	LYS	2.2
1	D	308	ILE	2.2
1	E	634	ASN	2.2
1	A	1059	LEU	2.2
1	C	709	GLU	2.2
1	F	372	ASP	2.2
1	C	753	THR	2.2
1	E	565	GLU	2.2
1	B	592	GLU	2.2
1	C	853	ASP	2.2
1	F	261	GLY	2.2
1	F	326	ALA	2.2
1	F	758	ASP	2.2
1	A	330	SER	2.2
1	C	800	ILE	2.1
1	A	217	VAL	2.1
1	B	663	GLU	2.1
1	C	402	GLU	2.1
1	F	39	MET	2.1
1	F	168	ASP	2.1
1	A	557	ARG	2.1
1	C	382	ARG	2.1
1	F	71	THR	2.1
1	F	761	ARG	2.1
1	E	716	GLU	2.1
1	C	115	ASN	2.1
1	C	808	GLU	2.1
1	D	471	GLU	2.1
1	F	653	ASP	2.1
1	F	557	ARG	2.1
1	A	565	GLU	2.1
1	E	663	GLU	2.1
1	E	400	PHE	2.1
1	C	186	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	326	ALA	2.1
1	D	935	TYR	2.1
1	C	165	VAL	2.1
1	D	614	PRO	2.1
1	D	297	ASN	2.1
1	F	772	ASP	2.1
1	B	561	SER	2.1
1	F	1041	LEU	2.1
1	C	89	ASP	2.1
1	C	263	ASP	2.1
1	D	774	ASP	2.1
1	F	265	ARG	2.1
1	F	592	GLU	2.1
1	F	707	ALA	2.1
1	F	400	PHE	2.1
1	C	49	HIS	2.1
1	A	663	GLU	2.0
1	C	592	GLU	2.0
1	C	712	GLU	2.0
1	A	641	LEU	2.0
1	B	199	LEU	2.0
1	D	39	MET	2.0
1	A	705	ALA	2.0
1	F	49	HIS	2.0
1	C	265	ARG	2.0
1	C	269	SER	2.0
1	E	937	ASN	2.0
1	D	683	HIS	2.0
1	F	304	GLU	2.0
1	B	329	PHE	2.0
1	A	299	ASP	2.0
1	C	1017	ASP	2.0
1	D	382	ARG	2.0
1	D	569	ASN	2.0
1	E	667	ASP	2.0
1	F	382	ARG	2.0
1	B	67	LYS	2.0
1	E	561	SER	2.0
1	F	805	TYR	2.0
1	A	924	ILE	2.0
1	C	321	ILE	2.0
1	F	138	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	627	ARG	2.0
1	E	97	VAL	2.0
1	F	334	GLY	2.0
1	F	395	GLY	2.0
1	F	799	GLY	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 monosaccharides 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.