Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2025 – 10:04 AM EDT

PDB ID	:	1K32 / pdb_00001k32
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 (i) 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 (i)) were used in the production of this report:

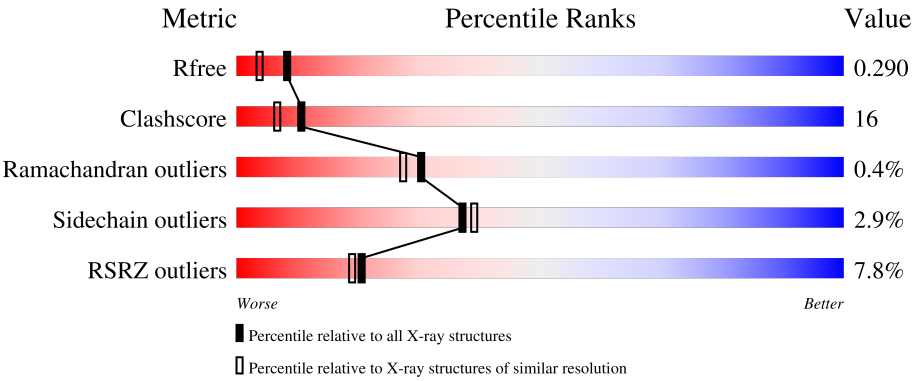
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 <=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	5% 70% 25%
1	B	1045	6% 68% 27%
1	C	1045	11% 67% 28%
1	D	1045	7% 71% 24%
1	E	1045	6% 71% 24%

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Mol	Chain	Length	Quality of chain
1	F	1045	

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
1	A	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	B	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	C	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	D	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	E	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			
1	F	1023	Total	C	N	O	S	95	0	0
			8177	5196	1402	1551	28			

- Molecule 2 is water.

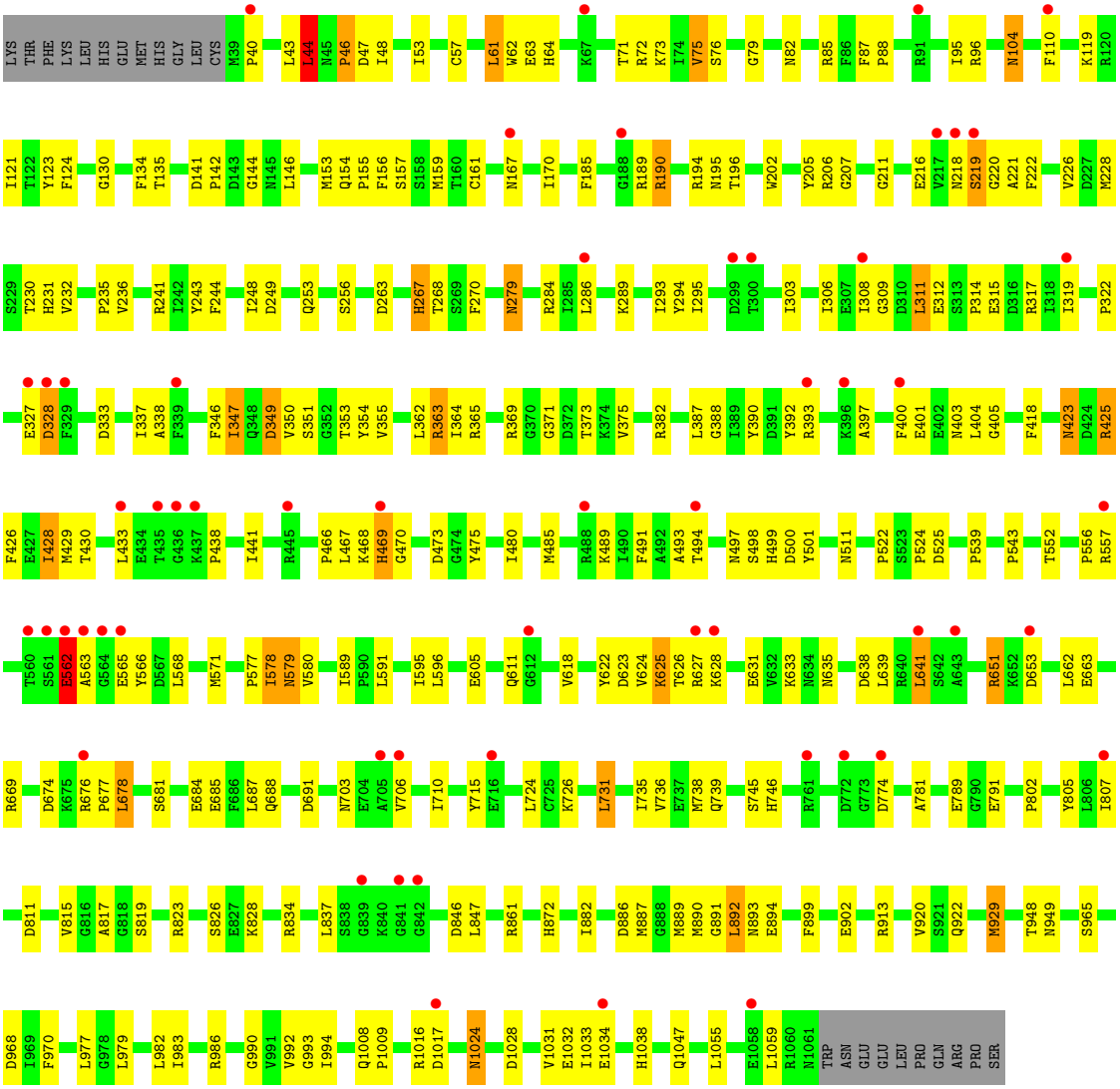
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	401	Total	O	0	0
			401	401		
2	B	395	Total	O	0	0
			395	395		
2	C	398	Total	O	0	0
			398	398		
2	D	401	Total	O	0	0
			401	401		
2	E	405	Total	O	0	0
			405	405		
2	F	394	Total	O	0	0
			394	394		

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.

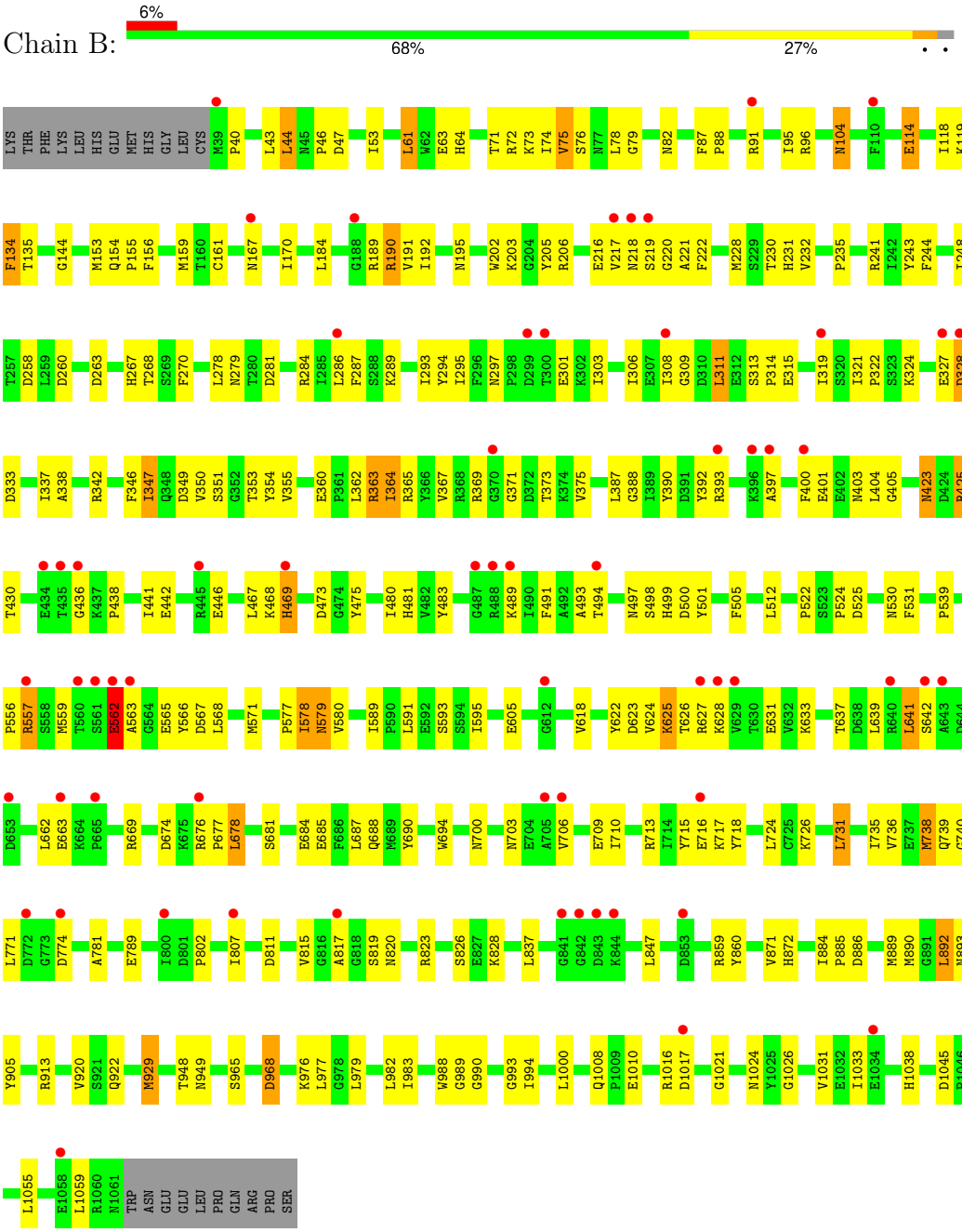
• Molecule 1: tricorn protease

Chain A:



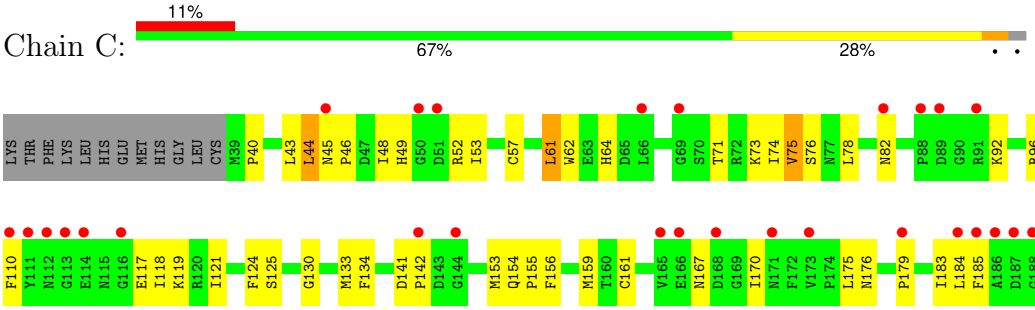
• Molecule 1: tricorn protease

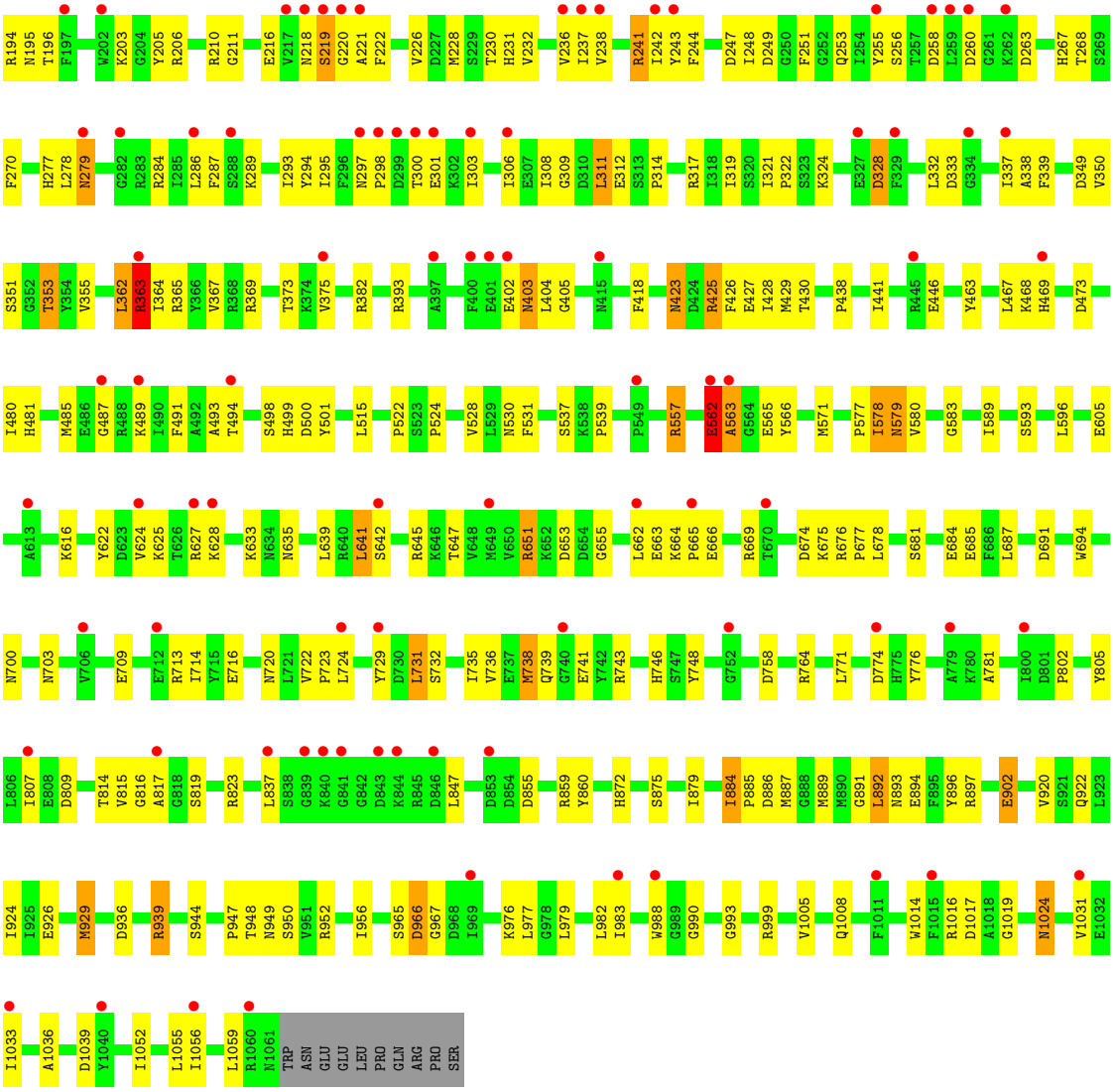
Chain B:



• Molecule 1: tricorn protease

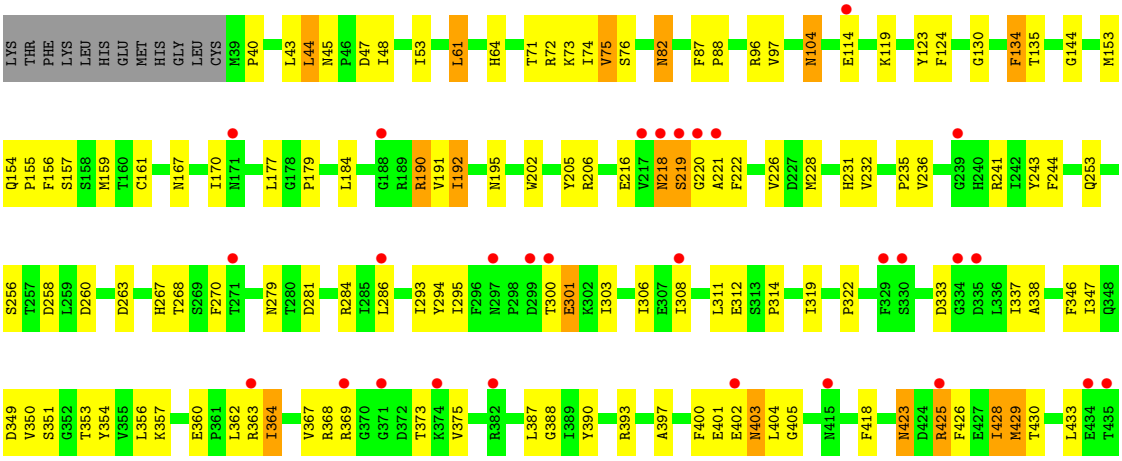
Chain C:

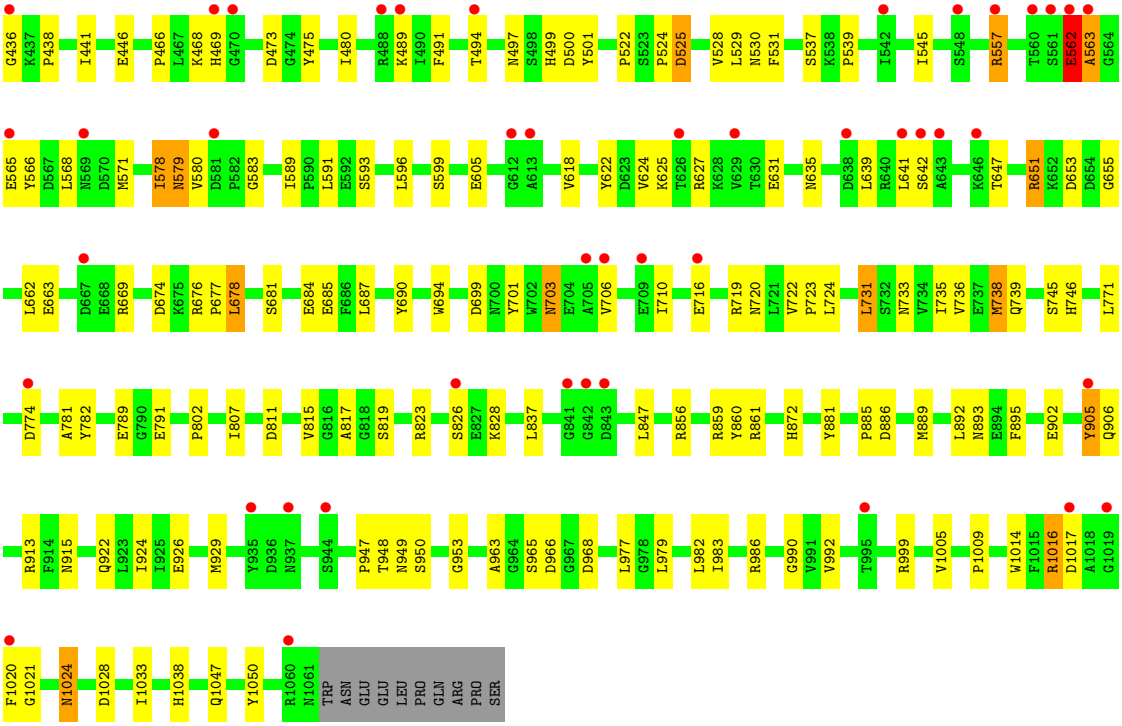




• Molecule 1: tricorn protease

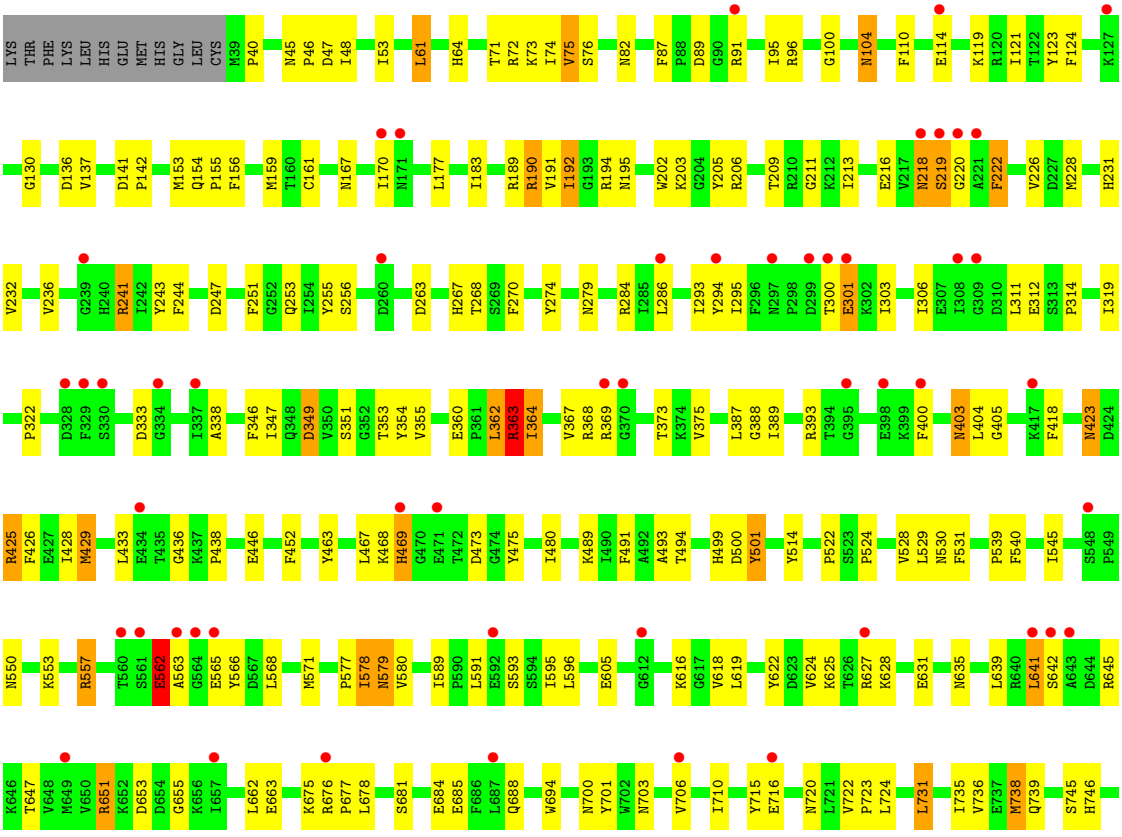
Chain D:

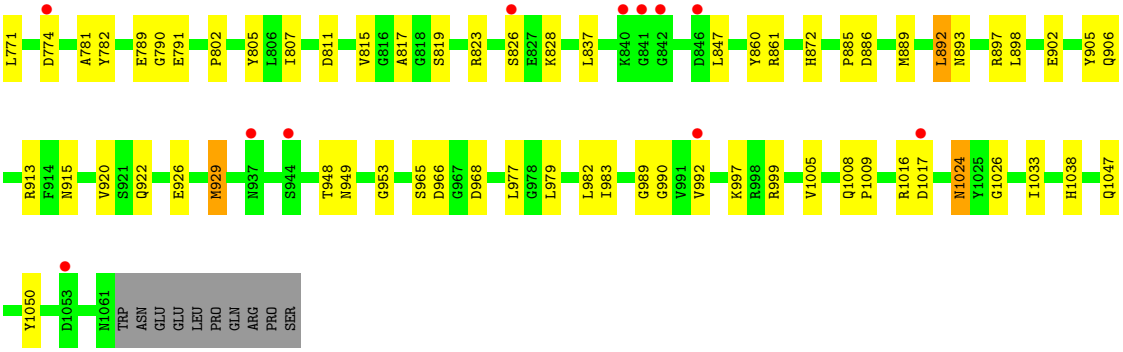




• Molecule 1: tricorn protease

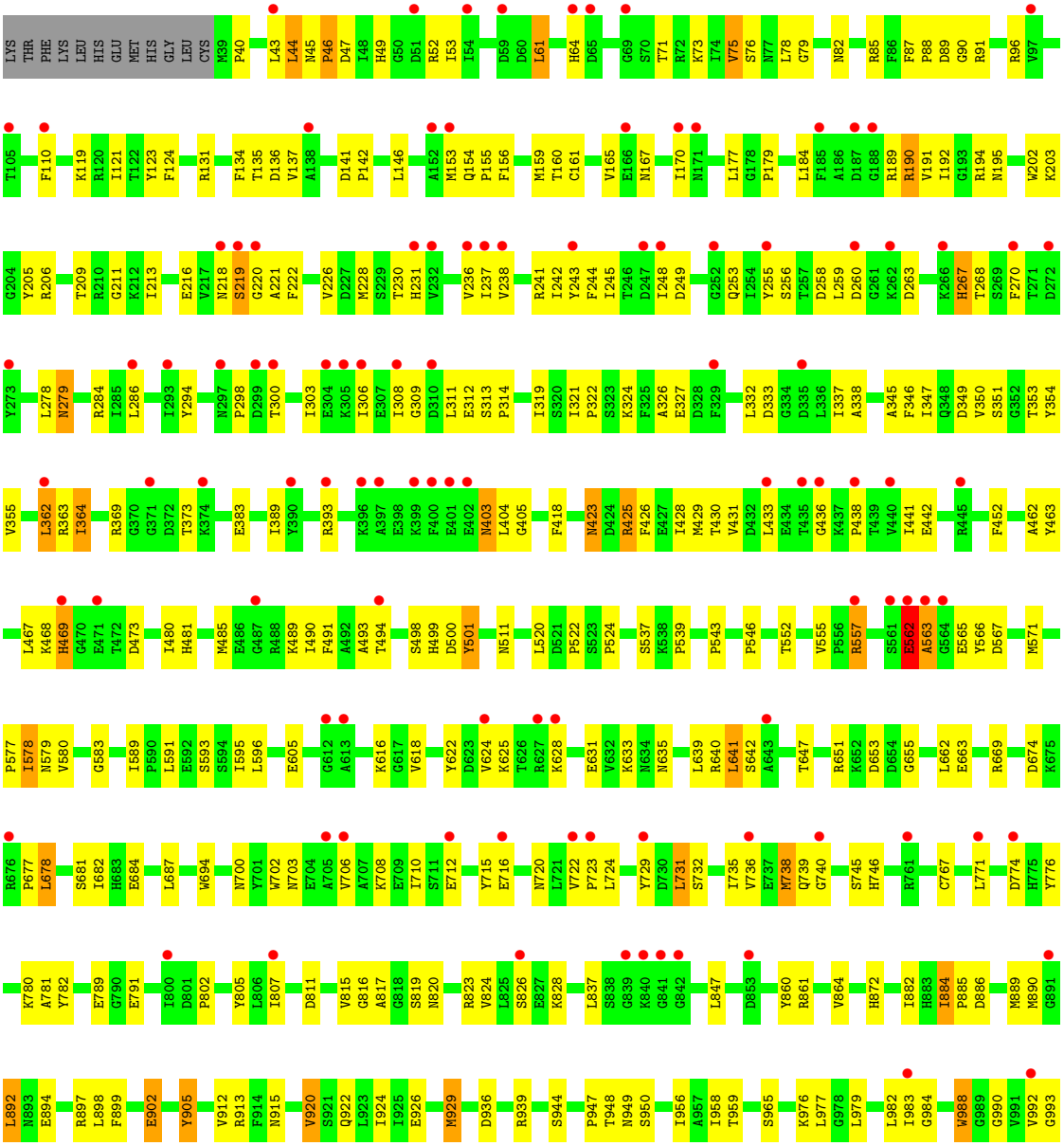
Chain E:

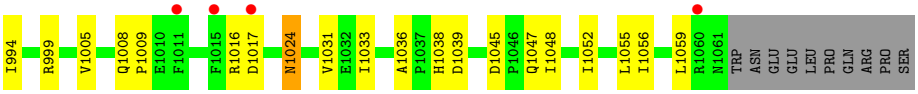




• Molecule 1: tricorn protease

Chain F:




I994
R999
V1005
Q1008
P1009
E1010
F1011
F1015
R1016
D1017
N1024
V1031
E1032
I1033
A1036
P1037
H1038
D1039
D1045
P1046
Q1047
I1048
I1052
L1055
I1056
L1059
R1060
N1061
TRP
ASN
GLU
GLU
LEU
PRO
GLN
ARG
PRO
SER

4 Data and refinement statistics (i)

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 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	78.6 (20.00-2.00) 82.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.264 0.253 , 0.290	Depositor DCC
R_{free} test set	19826 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/8367	0.93	22/11311 (0.2%)
1	B	0.47	0/8367	0.93	31/11311 (0.3%)
1	C	0.40	0/8367	0.93	25/11311 (0.2%)
1	D	0.45	0/8367	0.93	27/11311 (0.2%)
1	E	0.44	0/8367	0.93	25/11311 (0.2%)
1	F	0.40	0/8367	0.92	22/11311 (0.2%)
All	All	0.44	0/50202	0.93	152/67866 (0.2%)

There are no bond length outliers.

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	362	LEU	N-CA-C	9.49	123.62	110.24
1	C	364	ILE	N-CA-C	-9.41	94.25	107.99
1	A	362	LEU	N-CA-C	9.33	123.39	110.24
1	D	362	LEU	N-CA-C	8.70	122.51	110.24
1	C	362	LEU	N-CA-C	8.55	121.36	110.24
1	E	364	ILE	N-CA-C	-8.47	96.39	108.58
1	F	884	ILE	CA-C-N	8.21	128.17	119.05
1	F	884	ILE	C-N-CA	8.21	128.17	119.05
1	E	362	LEU	N-CA-C	8.19	121.79	110.24
1	A	364	ILE	N-CA-C	-8.12	95.81	108.23
1	C	363	ARG	N-CA-C	8.08	120.36	110.91
1	F	362	LEU	N-CA-C	8.06	120.71	110.24
1	C	884	ILE	CA-C-N	8.01	128.09	119.28
1	C	884	ILE	C-N-CA	8.01	128.09	119.28
1	C	425	ARG	N-CA-C	-8.00	103.52	113.28
1	B	364	ILE	N-CA-C	-7.73	97.10	108.54
1	F	425	ARG	N-CA-C	-7.70	103.61	113.16
1	B	968	ASP	N-CA-C	-7.65	102.88	111.14
1	C	993	GLY	N-CA-C	7.64	120.73	112.33
1	D	364	ILE	N-CA-C	-7.42	96.87	108.23
1	B	79	GLY	N-CA-C	-7.34	99.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	425	ARG	N-CA-C	-7.29	104.38	113.28
1	E	425	ARG	N-CA-C	-7.19	104.50	113.28
1	F	364	ILE	N-CA-C	-7.16	97.28	108.23
1	B	1021	GLY	N-CA-C	7.07	122.67	113.27
1	B	425	ARG	N-CA-C	-6.87	104.90	113.28
1	A	425	ARG	N-CA-C	-6.83	104.95	113.28
1	F	993	GLY	N-CA-C	6.81	119.82	112.33
1	A	428	ILE	N-CA-C	-6.76	98.75	108.48
1	C	428	ILE	N-CA-C	-6.75	98.66	108.11
1	A	79	GLY	N-CA-C	-6.57	101.01	110.60
1	A	715	TYR	N-CA-C	6.56	119.02	111.02
1	B	905	TYR	N-CA-C	-6.51	101.15	110.59
1	D	966	ASP	N-CA-C	-6.49	104.47	112.38
1	B	746	HIS	N-CA-C	6.43	120.42	112.58
1	A	746	HIS	N-CA-C	6.38	120.37	112.58
1	A	968	ASP	N-CA-C	-6.37	104.26	111.14
1	C	675	LYS	N-CA-C	-6.35	104.44	111.36
1	C	746	HIS	N-CA-C	6.33	120.15	111.54
1	E	100	GLY	N-CA-C	-6.29	103.75	112.18
1	D	349	ASP	N-CA-C	-6.29	102.42	110.53
1	D	746	HIS	N-CA-C	6.26	120.19	111.74
1	E	349	ASP	N-CA-C	-6.23	102.49	110.53
1	E	301	GLU	N-CA-C	-6.17	105.71	113.23
1	B	674	ASP	N-CA-C	6.16	119.75	112.72
1	A	497	ASN	N-CA-C	6.16	120.79	113.28
1	B	428	ILE	N-CA-C	-6.12	99.66	108.48
1	E	746	HIS	N-CA-C	6.07	119.94	111.74
1	C	349	ASP	N-CA-C	-6.00	101.88	110.59
1	F	905	TYR	N-CA-C	-5.93	101.99	110.59
1	E	847	LEU	N-CA-C	5.92	118.86	109.50
1	A	651	ARG	N-CA-C	-5.92	100.07	109.59
1	D	651	ARG	N-CA-C	-5.89	99.30	108.90
1	B	651	ARG	N-CA-C	-5.88	99.61	109.07
1	B	847	LEU	N-CA-C	5.88	119.12	109.72
1	E	651	ARG	N-CA-C	-5.87	99.33	108.90
1	D	1021	GLY	N-CA-C	5.85	120.89	114.40
1	D	301	GLU	N-CA-C	-5.85	106.09	113.23
1	A	196	THR	N-CA-C	5.79	119.87	113.21
1	F	920	VAL	N-CA-C	5.78	117.72	112.29
1	D	134	PHE	N-CA-C	5.77	117.97	110.53
1	D	428	ILE	N-CA-C	-5.75	100.06	108.11
1	E	966	ASP	N-CA-C	-5.75	105.36	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	905	TYR	N-CA-C	-5.72	101.50	110.36
1	E	428	ILE	N-CA-C	-5.71	99.89	108.12
1	E	715	TYR	N-CA-C	5.70	117.97	111.02
1	C	277	HIS	N-CA-C	5.67	118.11	111.02
1	F	355	VAL	N-CA-C	5.67	116.05	108.11
1	D	192	ILE	N-CA-C	5.65	116.08	108.17
1	B	134	PHE	N-CA-C	5.64	118.17	110.55
1	C	748	TYR	N-CA-C	5.64	118.43	110.14
1	B	716	GLU	N-CA-C	5.63	117.09	111.07
1	F	428	ILE	N-CA-C	-5.63	100.23	108.11
1	F	78	LEU	N-CA-C	-5.61	106.32	114.12
1	F	902	GLU	N-CA-C	5.60	120.80	113.30
1	C	952	ARG	N-CA-C	5.59	117.37	111.28
1	F	79	GLY	N-CA-C	-5.59	105.92	111.56
1	C	44	LEU	N-CA-C	5.57	116.73	108.60
1	C	847	LEU	N-CA-C	5.57	118.30	109.50
1	C	902	GLU	N-CA-C	5.56	120.18	113.17
1	A	847	LEU	N-CA-C	5.56	118.61	109.72
1	A	349	ASP	N-CA-C	-5.55	103.37	110.53
1	D	674	ASP	N-CA-C	5.54	119.04	112.72
1	D	847	LEU	N-CA-C	5.54	118.25	109.50
1	C	939	ARG	N-CA-C	-5.53	105.25	111.28
1	D	699	ASP	N-CA-C	5.53	118.07	111.71
1	B	192	ILE	N-CA-C	5.53	115.81	107.80
1	D	497	ASN	N-CA-C	5.53	120.02	113.28
1	A	87	PHE	N-CA-C	-5.53	102.24	110.20
1	B	87	PHE	N-CA-C	-5.52	102.11	110.39
1	A	267	HIS	N-CA-C	5.51	120.12	113.17
1	F	349	ASP	N-CA-C	-5.51	102.60	110.59
1	F	715	TYR	N-CA-C	5.51	117.74	111.02
1	B	884	ILE	CA-C-N	5.50	125.02	119.19
1	B	884	ILE	C-N-CA	5.50	125.02	119.19
1	B	715	TYR	N-CA-C	5.50	117.73	111.02
1	E	87	PHE	N-CA-C	-5.49	102.05	110.07
1	C	355	VAL	N-CA-C	5.46	116.35	108.48
1	A	347	ILE	N-CA-C	-5.45	100.48	108.11
1	E	782	TYR	N-CA-C	5.45	118.81	110.20
1	C	487	GLY	N-CA-C	-5.41	107.56	114.37
1	D	44	LEU	N-CA-C	5.41	117.02	108.96
1	A	47	ASP	N-CA-C	-5.40	101.09	109.24
1	D	1016	ARG	N-CA-C	-5.38	102.08	110.10
1	B	993	GLY	N-CA-C	5.37	120.73	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	196	THR	N-CA-C	5.36	119.37	113.21
1	A	95	ILE	N-CA-C	5.35	116.43	108.46
1	E	95	ILE	N-CA-C	5.32	115.78	108.12
1	B	281	ASP	N-CA-C	-5.32	106.02	112.88
1	A	44	LEU	N-CA-C	5.30	116.86	108.96
1	A	993	GLY	N-CA-C	5.29	120.61	112.51
1	D	47	ASP	N-CA-C	-5.29	101.03	109.07
1	D	87	PHE	N-CA-C	-5.27	102.48	110.39
1	B	44	LEU	N-CA-C	5.26	116.97	109.14
1	E	222	PHE	N-CA-C	5.25	117.96	109.40
1	D	782	TYR	N-CA-C	5.25	118.49	110.20
1	B	347	ILE	N-CA-C	-5.24	100.77	108.11
1	F	501	TYR	N-CA-C	5.24	115.97	108.74
1	D	525	ASP	N-CA-C	-5.23	102.54	110.28
1	E	501	TYR	N-CA-C	5.21	115.02	108.45
1	E	905	TYR	N-CA-C	-5.20	102.30	110.36
1	D	281	ASP	N-CA-C	-5.20	106.17	112.88
1	E	192	ILE	N-CA-C	5.19	115.33	107.75
1	A	674	ASP	N-CA-C	5.19	118.92	112.59
1	E	675	LYS	N-CA-C	-5.18	105.81	111.82
1	B	1010	GLU	N-CA-C	5.17	119.86	113.50
1	C	651	ARG	N-CA-C	-5.17	100.75	109.07
1	B	1000	LEU	N-CA-C	-5.14	103.90	110.53
1	C	501	TYR	N-CA-C	5.13	115.31	108.38
1	F	267	HIS	N-CA-C	5.13	119.52	113.16
1	B	95	ILE	N-CA-C	5.11	116.07	108.46
1	B	497	ASN	N-CA-C	5.10	119.51	113.28
1	C	134	PHE	N-CA-C	5.10	117.11	110.53
1	B	525	ASP	N-CA-C	-5.10	102.74	110.28
1	E	47	ASP	N-CA-C	-5.09	101.33	109.07
1	F	555	VAL	N-CA-C	-5.09	103.97	108.95
1	B	902	GLU	N-CA-C	5.08	120.32	113.72
1	D	963	ALA	N-CA-C	-5.07	101.44	109.76
1	B	349	ASP	N-CA-C	-5.07	103.99	110.53
1	C	966	ASP	N-CA-C	-5.06	106.80	112.87
1	B	47	ASP	N-CA-C	-5.05	101.61	109.24
1	F	847	LEU	N-CA-C	5.05	117.48	109.50
1	F	988	TRP	N-CA-C	5.04	117.16	111.11
1	E	363	ARG	N-CA-C	5.04	121.54	110.80
1	E	545	ILE	CA-C-N	5.03	124.94	119.76
1	E	545	ILE	C-N-CA	5.03	124.94	119.76
1	F	746	HIS	N-CA-C	5.03	118.53	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	525	ASP	N-CA-C	-5.02	102.27	110.20
1	F	702	TRP	N-CA-C	5.01	117.40	111.33
1	E	355	VAL	N-CA-C	5.01	115.12	108.11
1	D	545	ILE	CA-C-N	5.00	125.00	119.90
1	D	545	ILE	C-N-CA	5.00	125.00	119.90

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	274	0
1	B	8177	0	8003	283	0
1	C	8177	0	8003	298	0
1	D	8177	0	8003	245	0
1	E	8177	0	8003	265	0
1	F	8177	0	8003	298	0
2	A	401	0	0	12	0
2	B	395	0	0	10	0
2	C	398	0	0	18	0
2	D	401	0	0	10	0
2	E	405	0	0	11	0
2	F	394	0	0	11	0
All	All	51456	0	48018	1573	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 16.

All (1573) 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:155:PRO:HG2	1:B:159:MET:HE1	1.35	1.09
1:D:155:PRO:HG2	1:D:159:MET:HE1	1.33	1.06
1:B:983:ILE:HG23	1:B:1033:ILE:HD13	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HG2	1:A:159:MET:HE1	1.39	1.02
1:F:155:PRO:HG2	1:F:159:MET:HE1	1.41	1.01
1:C:155:PRO:HG2	1:C:159:MET:HE1	1.43	1.00
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:E:155:PRO:HG2	1:E:159:MET:HE1	1.46	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: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:B:155:PRO:CG	1:B:159:MET:HE1	2.02	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
1:B:480:ILE:H	1:B:494:THR:HG22	1.38	0.87
1:D:155:PRO:CG	1:D:159:MET:HE1	2.04	0.87
1:F:155:PRO:CG	1:F:159:MET:HE1	2.04	0.87
1:A:155:PRO:CG	1:A:159:MET:HE1	2.05	0.86
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:154:GLN:HB3	1:C:159:MET:HE3	1.57	0.85
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:E:228:MET:HE1	1:E:244:PHE:CE1	2.12	0.84
1:E:155:PRO:CG	1:E:159:MET:HE1	2.07	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:D:156:PHE:HD1	1:D:159:MET:HE2	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:929:MET:HE2	1:D:929:MET:HA	1.61	0.82
1:C:155:PRO:CG	1:C:159:MET:HE1	2.09	0.82
1:D:104:ASN:H	1:D:104:ASN:HD22	1.26	0.82
1:C:929:MET:HE2	1:C:929:MET:HA	1.61	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:D:228:MET:HE1	1:D:244:PHE:CE1	2.16	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:B:228:MET:HE1	1:B:244:PHE:CE1	2.15	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:E:154:GLN:HB3	1:E:159:MET:HE3	1.62	0.80
1:E:568:LEU:HB3	1:E:571:MET:HE2	1.63	0.80
1:D:48:ILE:HB	1:D:286:LEU:HD22	1.64	0.79
1:F:154:GLN:HB3	1:F:159:MET:HE3	1.62	0.79
1:E:156:PHE:HD1	1:E:159:MET:HE2	1.46	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:228:MET:HE1	1:A:244:PHE:CE1	2.19	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:A:948:THR:H	1:B:922:GLN:NE2	1.82	0.78
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
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:D:156:PHE:CD1	1:D:159:MET:HE2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:156:PHE:CD1	1:E:159:MET:HE2	2.21	0.76
1:F:694:TRP:HA	1:F:738:MET:HE1	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:A:429:MET:HE3	1:A:438:PRO:HB2	1.68	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:F:155:PRO:CD	1:F:159:MET:HE1	2.17	0.75
1:D:53:ILE:CG2	1:D:286:LEU:HD21	2.16	0.74
1:E:155:PRO:CD	1:E:159:MET:HE1	2.17	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:A:228:MET:HE3	1:A:232:VAL:CG2	2.19	0.73
1:F:206:ARG:H	1:F:1024:ASN:HD21	1.37	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:156:PHE:HD1	1:A:159:MET:HE2	1.55	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:D:703:ASN:C	1:D:703:ASN:HD22	1.98	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:228:MET:HE1	1:C:244:PHE:CE1	2.25	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:156:PHE:CD1	1:A:159:MET:HE2	2.25	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:E:403:ASN:HD22	1:E:403:ASN:C	1.99	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:A:155:PRO:CD	1:A:159:MET:HE1	2.22	0.69
1:B:156:PHE:HD1	1:B:159:MET:HE2	1.57	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:B:155:PRO:CD	1:B:159:MET:HE1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:THR:HG23	1:B:441:ILE:HD11	1.75	0.68
1:D:403:ASN:HD22	1:D:403:ASN:C	2.01	0.68
1:E:530:ASN:ND2	1:E:531:PHE:H	1.90	0.68
1:F:982:LEU:C	1:F:983:ILE:HD12	2.17	0.68
1:C:350:VAL:HG21	1:C:669:ARG:HH11	1.58	0.68
1:E:226:VAL:CG1	1:E:228:MET:HE2	2.24	0.68
1:B:156:PHE:CD1	1:B:159:MET:HE2	2.28	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:F:228:MET:HE1	1:F:244:PHE:CE1	2.29	0.67
1:B:404:LEU:HD22	1:B:429:MET:CE	2.24	0.67
1:C:403:ASN:HD22	1:C:403:ASN:C	2.03	0.67
1:A:350:VAL:HG21	1:A:669:ARG:NH1	2.10	0.67
1:B:154:GLN:HB3	1:B:159:MET:HE3	1.77	0.67
1:E:190:ARG:NH2	1:E:222:PHE:HZ	1.93	0.67
1:E:929:MET:HA	1:E:929:MET:HE2	1.76	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:B:404:LEU:HD22	1:B:429:MET:HE1	1.77	0.66
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:C:155:PRO:CD	1:C:159:MET:HE1	2.26	0.66
1:D:913:ARG:HH21	1:D:1047:GLN:HE21	1.42	0.66
1:C:929:MET:HE3	1:C:979:LEU:CD1	2.25	0.66
1:D:480:ILE:H	1:D:494:THR:HG22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:423:ASN:HD22	1:F:423:ASN:C	2.04	0.66
1:A:522:PRO:HD3	1:B:893:ASN:OD1	1.95	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:E:404:LEU:HD22	1:E:429:MET:HE1	1.79	0.65
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.26	0.65
1:C:156:PHE:HD1	1:C:159:MET:HE2	1.61	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:C:423:ASN:C	1:C:423:ASN:HD22	2.04	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:B:228:MET:HE3	1:B:232:VAL:HG22	1.79	0.64
1:B:929:MET:HA	1:B:929:MET:HE2	1.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HB2	1:A:286:LEU:HD21	1.80	0.64
1:A:154:GLN:HB3	1:A:159:MET:HE3	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
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: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:A:789:GLU:OE2	2:A:2230:HOH:O	2.15	0.63
1:C:228:MET:HE1	1:C:244:PHE:CZ	2.34	0.63
1:D:404:LEU:HD22	1:D:429:MET:HE1	1.81	0.63
1:B:929:MET:HE3	1:B:979:LEU:CD1	2.28	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:A:889:MET:SD	1:B:522:PRO:HG2	2.38	0.63
1:E:333:ASP:CG	1:E:369:ARG:HE	2.06	0.63
1:F:403:ASN:HD22	1:F:403:ASN:C	2.07	0.63
1:E:312:GLU:HG2	1:E:314:PRO:HD3	1.80	0.63
1:F:404:LEU:HD22	1:F:429:MET:CE	2.28	0.63
1:F:418:PHE:CE1	1:F:485:MET:HE2	2.33	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:228:MET:HE3	1:B:232:VAL:CG2	2.29	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:494:THR:HG21	1:D:500:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:218:ASN:O	1:F:219:SER:C	2.43	0.62
1:E:694:TRP:HA	1:E:738:MET:HE1	1.82	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
1:F:999:ARG:HG2	1:F:1005:VAL:HG22	1.81	0.62
1:A:346:PHE:C	1:A:347:ILE:HD12	2.25	0.61
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:D:228:MET:HE3	1:D:232:VAL:CG2	2.30	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:F:228:MET:HE1	1:F:244:PHE:CZ	2.35	0.61
1:A:403:ASN:ND2	1:A:405:GLY:H	1.97	0.61
1:D:226:VAL:CG1	1:D:228:MET:HE2	2.31	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: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:C:694:TRP:HA	1:C:738:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:PRO:HG2	1:F:159:MET:CE	2.25	0.61
1:F:156:PHE:HD1	1:F:159:MET:HE2	1.66	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:124:PHE:CE2	1:B:153:MET:HE1	2.35	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:423:ASN:C	1:A:423:ASN:HD22	2.09	0.60
1:A:662:LEU:HD23	1:A:662:LEU:O	2.02	0.60
1:A:929:MET:HE2	1:A:929:MET:HA	1.81	0.60
1:F:156:PHE:CD1	1:F:159:MET:HE2	2.37	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:D:155:PRO:CD	1:D:159:MET:HE1	2.30	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: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:156:PHE:CD1	1:C:159:MET:HE2	2.37	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
1:A:256:SER:OG	1:A:267:HIS:HE1	1.84	0.60
1:B:322:PRO:HB3	1:B:678:LEU:HD13	1.83	0.59
1:B:423:ASN:C	1:B:423:ASN:HD22	2.09	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:F:258:ASP:C	1:F:260:ASP:H	2.10	0.59
1:C:309:GLY:O	1:C:311:LEU:HD13	2.03	0.59
1:D:346:PHE:C	1:D:347:ILE:HD12	2.27	0.59
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:MET:HE3	1:E:232:VAL:CG2	2.32	0.59
1:E:429:MET:HE3	1:E:438:PRO:CB	2.32	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:228:MET:HE1	1:B:244:PHE:HE1	1.67	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: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: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:E:228:MET:HE3	1:E:232:VAL:HG22	1.83	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:A:228:MET:HE3	1:A:232:VAL:HG21	1.85	0.58
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:F:929:MET:HE2	1:F:929:MET:HA	1.85	0.58
1:B:703:ASN:HD22	1:B:703:ASN:C	2.12	0.58
1:D:190:ARG:NH2	1:D:216:GLU:OE2	2.35	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:429:MET:HE3	1:E:438:PRO:HB2	1.84	0.58
1:A:226:VAL:HG13	1:A:228:MET:HE2	1.84	0.58
1:C:43:LEU:O	1:C:44:LEU:HG	2.04	0.58
1:C:694:TRP:HA	1:C:738:MET:HE2	1.84	0.58
1:D:872:HIS:HE1	1:D:902:GLU:OE1	1.86	0.58
1:A:703:ASN:C	1:A:703:ASN:HD22	2.11	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:B:982:LEU:C	1:B:983:ILE:HD12	2.29	0.57
1:D:635:ASN:HB3	1:D:653:ASP:OD1	2.04	0.57
1:F:404:LEU:HD22	1:F:429:MET:HE2	1.86	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:947:PRO:HD2	1:F:950:SER:HB3	1.85	0.57
1:D:429:MET:HE3	1:D:438:PRO:HB2	1.86	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:B:351:SER:HG	1:B:353:THR:HG22	1.70	0.57
1:E:815:VAL:HA	1:E:819:SER:HB3	1.86	0.57
1:C:230:THR:HG21	1:C:248:ILE:HA	1.87	0.57
1:C:333:ASP:CG	1:C:369:ARG:HE	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:684:GLU:HG3	1:D:685:GLU:N	2.19	0.57
1:A:982:LEU:C	1:A:983:ILE:HD12	2.30	0.56
1:B:467:LEU:C	1:B:467:LEU:HD12	2.29	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:D:929:MET:HE3	1:D:979:LEU:HG	1.87	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:333:ASP:CG	1:D:369:ARG:HE	2.12	0.56
1:D:360:GLU:HB2	1:D:364:ILE:HD11	1.86	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:B:929:MET:HE3	1:B:979:LEU:HD11	1.88	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: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:C:418:PHE:CE1	1:C:485:MET:HE2	2.40	0.56
1:F:312:GLU:HG2	1:F:314:PRO:HD3	1.87	0.56
1:C:703:ASN:C	1:C:703:ASN:HD22	2.13	0.56
1:D:999:ARG:HG2	1:D:1005:VAL:HG22	1.86	0.56
1:F:562:GLU:O	1:F:563:ALA:HB3	2.06	0.56
1:F:965:SER:HA	1:F:990:GLY:O	2.06	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: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:872:HIS:HE1	1:E:902:GLU:OE1	1.89	0.56
1:A:226:VAL:CG1	1:A:228:MET:HE2	2.36	0.56
1:D:568:LEU:HB3	1:D:571:MET:HE2	1.87	0.56
1:E:155:PRO:HD2	1:E:159:MET:HE1	1.87	0.56
1:E:228:MET:HE1	1:E:244:PHE:CZ	2.40	0.56
1:E:1016:ARG:O	1:E:1017:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:703:ASN:C	1:E:703:ASN:HD22	2.13	0.55
1:F:635:ASN:HB3	1:F:653:ASP:OD1	2.07	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: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:E:494:THR:HG21	1:E:500:ASP:OD1	2.07	0.55
1:A:929:MET:HE3	1:A:979:LEU:CD1	2.37	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:F:429:MET:HE3	1:F:438:PRO:HB2	1.89	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:D:154:GLN:HB3	1:D:159:MET:HE3	1.87	0.54
1:D:295:ILE:HG13	1:D:306:ILE:HD11	1.87	0.54
1:B:403:ASN:HD22	1:B:403:ASN:C	2.16	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:333:ASP:CG	1:F:369:ARG:HE	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:639:LEU:HD23	1:F:639:LEU:C	2.33	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:530:ASN:ND2	1:E:531:PHE:N	2.55	0.54
1:F:346:PHE:C	1:F:347:ILE:HD12	2.32	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: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: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:218:ASN:O	1:C:219:SER:C	2.50	0.54
1:C:562:GLU:O	1:C:563:ALA:HB3	2.08	0.54
1:E:346:PHE:C	1:E:347:ILE:HD12	2.33	0.54
1:C:206:ARG:H	1:C:1024:ASN:ND2	2.06	0.54
1:C:228:MET:HE3	1:C:232:VAL:CG2	2.38	0.54
1:D:64:HIS:HD2	1:D:71:THR:OG1	1.91	0.54
1:D:104:ASN:H	1:D:104:ASN:ND2	2.00	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:B:155:PRO:HD2	1:B:159:MET:HE1	1.90	0.53
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:429:MET:HE3	1:A:438:PRO:CB	2.37	0.53
1:A:494:THR:HG21	1:A:500:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ARG:HH22	1:F:557:ARG:NE	2.06	0.53
1:F:155:PRO:HD2	1:F:159:MET:HE1	1.87	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:D:429:MET:HE3	1:D:438:PRO:CB	2.38	0.53
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.55	0.53
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: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:639:LEU:HD23	1:C:639:LEU:C	2.33	0.53
1:C:929:MET:HA	1:C:929:MET:CE	2.36	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:D:124:PHE:CE2	1:D:153:MET:HE1	2.44	0.53
1:D:155:PRO:HG2	1:D:159:MET:CE	2.22	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: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:B:639:LEU:C	1:B:639:LEU:HD23	2.34	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:A:791:GLU:CD	1:A:861:ARG:HE	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:404:LEU:HD22	1:A:429:MET:HE2	1.90	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
1:C:404:LEU:HD22	1:C:429:MET:HE1	1.91	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:F:1052:ILE:O	1:F:1056:ILE:HG13	2.10	0.52
1:B:429:MET:HE3	1:B:438:PRO:HB2	1.90	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:A:351:SER:HG	1:A:353:THR:HG22	1.72	0.52
1:C:249:ASP:HB2	2:C:4014:HOH:O	2.08	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:676:ARG:HD2	2:C:4370:HOH:O	2.08	0.52
1:D:228:MET:HE3	1:D:232:VAL:HG22	1.91	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:D:557:ARG:HD2	1:F:393:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:VAL:HG22	1:A:622:TYR:CD2	2.44	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
1:C:982:LEU:C	1:C:983:ILE:HD12	2.35	0.52
1:A:206:ARG:N	1:A:1024:ASN:HD21	2.07	0.52
1:A:327:GLU:O	1:A:328:ASP:C	2.53	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:694:TRP:HA	1:D:738:MET:HE2	1.92	0.52
1:D:885:PRO:O	1:D:915:ASN:HA	2.09	0.52
1:E:226:VAL:HG13	1:E:228:MET:HE2	1.91	0.52
1:F:791:GLU:CD	1:F:861:ARG:HE	2.18	0.52
1:A:475:TYR:OH	1:B:949:ASN:ND2	2.43	0.51
1:B:155:PRO:HG2	1:B:159:MET:CE	2.25	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: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: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:A:155:PRO:HD2	1:A:159:MET:HE1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:124:PHE:CE2	1:C:153:MET:HE1	2.45	0.51
1:E:423:ASN:C	1:E:423:ASN:HD22	2.18	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: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:F:156:PHE:H	1:F:159:MET:CE	2.24	0.50
1:C:929:MET:HE3	1:C:979:LEU:HG	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ILE:HB	1:A:286:LEU:HD22	1.94	0.50
1:A:403:ASN:HD22	1:A:403:ASN:C	2.18	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:E:467:LEU:HD12	1:E:467:LEU:C	2.37	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:A:124:PHE:CE2	1:A:153:MET:HE1	2.47	0.50
1:B:872:HIS:CE1	1:B:902:GLU:OE1	2.65	0.50
1:E:124:PHE:CE2	1:E:153:MET:HE1	2.47	0.50
1:E:618:VAL:HG21	1:E:631:GLU:HG3	1.94	0.50
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:A:404:LEU:HD22	1:A:429:MET:CE	2.42	0.50
1:A:418:PHE:CE1	1:A:485:MET:HE2	2.47	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: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:616:LYS:HE2	1:F:653:ASP:CB	2.42	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:D:929:MET:HE3	1:D:979:LEU:CD1	2.42	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: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:A:605:GLU:HG2	1:B:524:PRO:HD3	1.93	0.49
1:A:639:LEU:HD23	1:A:639:LEU:C	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ARG:NH2	1:C:365:ARG:HH22	2.11	0.49
1:D:929:MET:HA	1:D:929:MET:CE	2.36	0.49
1:E:46:PRO:HB2	1:E:286:LEU:HD23	1.94	0.49
1:E:155:PRO:HG2	1:E:159:MET:CE	2.32	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: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:B:104:ASN:HD22	1:B:104:ASN:N	1.93	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
1:B:286:LEU:HD11	1:B:293:ILE:HG22	1.94	0.49
1:C:641:LEU:HD22	1:C:645:ARG:HA	1.94	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:134:PHE:O	1:B:135:THR:HB	2.12	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:738:MET:SD	1:F:738:MET:C	2.96	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: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:43:LEU:C	1:A:44:LEU:HG	2.38	0.48
1:A:218:ASN:O	1:A:219:SER:C	2.55	0.48
1:A:882:ILE:HD11	1:A:899:PHE:HA	1.94	0.48
1:C:155:PRO:HG2	1:C:159:MET:CE	2.30	0.48
1:C:156:PHE:HD1	1:C:159:MET:CE	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ILE:HG22	1:C:338:ALA:N	2.28	0.48
1:E:218:ASN:O	1:E:219:SER:C	2.56	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: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
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:D:218:ASN:O	1:D:219:SER:C	2.57	0.48
1:E:89:ASP:CG	1:E:91:ARG:HG3	2.38	0.48
1:E:639:LEU:C	1:E:639:LEU:HD23	2.39	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:965:SER:C	1:C:967:GLY:N	2.71	0.48
1:D:190:ARG:HH22	1:D:216:GLU:CD	2.21	0.48
1:D:228:MET:HE1	1:D:244:PHE:CZ	2.49	0.48
1:D:791:GLU:CD	1:D:861:ARG:HE	2.21	0.48
1:A:401:GLU:H	1:A:401:GLU:CD	2.20	0.48
1:A:499:HIS:HD2	2:A:2176:HOH:O	1.95	0.48
1:D:639:LEU:C	1:D:639:LEU:HD23	2.38	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:F:404:LEU:HD22	1:F:429:MET:HE1	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:HB3	1:A:221:ALA:HB3	1.95	0.48
1:A:228:MET:HE1	1:A:244:PHE:CZ	2.48	0.48
1:E:568:LEU:HB3	1:E:571:MET:CE	2.39	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:A:333:ASP:CG	1:A:369:ARG:HE	2.22	0.47
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:771:LEU:HD13	1:D:771:LEU:C	2.39	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:327:GLU:O	1:B:328:ASP:C	2.57	0.47
1:B:360:GLU:HB2	1:B:364:ILE:HD11	1.97	0.47
1:E:194:ARG:O	1:E:211:GLY:HA2	2.14	0.47
1:E:578:ILE:HD12	1:E:595:ILE:HD12	1.96	0.47
1:F:929:MET:HE3	1:F:979:LEU:CD1	2.45	0.47
1:A:314:PRO:HD2	1:A:726:LYS:HG2	1.94	0.47
1:B:218:ASN:O	1:B:219:SER:C	2.57	0.47
1:B:429:MET:HE3	1:B:438:PRO:CB	2.44	0.47
1:D:694:TRP:HA	1:D:738:MET:HE1	1.96	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:D:828:LYS:NZ	2:D:5341:HOH:O	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:241:ARG:HH12	1:F:263:ASP:CG	2.22	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:309:GLY:O	1:A:311:LEU:HD13	2.14	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:E:110:PHE:CD2	1:E:121:ILE:HG13	2.50	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:B:557:ARG:NH2	1:D:393:ARG:HH12	2.12	0.47
1:B:976:LYS:HZ3	1:B:1017:ASP:HB2	1.80	0.47
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:A:156:PHE:HB2	1:A:159:MET:HE2	1.96	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: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:D:982:LEU:C	1:D:983:ILE:HD12	2.39	0.47
1:E:562:GLU:O	1:E:563:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:469:HIS:HD1	1:F:473:ASP:CG	2.23	0.46
1:B:156:PHE:HB2	1:B:159:MET:HE2	1.96	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: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:226:VAL:CG1	1:C:228:MET:HE2	2.45	0.46
1:C:258:ASP:C	1:C:260:ASP:H	2.21	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:A:929:MET:HE3	1:A:979:LEU:HD11	1.98	0.46
1:D:222:PHE:H	1:D:1038:HIS:CD2	2.34	0.46
1:D:226:VAL:HG13	1:D:228:MET:HE2	1.96	0.46
1:D:703:ASN:C	1:D:703:ASN:ND2	2.71	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:203:LYS:HD3	1:F:740:GLY:C	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:155:PRO:HD2	1:C:159:MET:HE1	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:MET:HE3	1:E:438:PRO:HB3	1.98	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: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:700:ASN:HD22	1:B:1008:GLN:NE2	2.12	0.46
1:C:226:VAL:HG13	1:C:228:MET:HE2	1.98	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: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:B:333:ASP:CG	1:B:369:ARG:HE	2.24	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:F:226:VAL:HG13	1:F:228:MET:HE2	1.98	0.46
1:B:404:LEU:HD22	1:B:429:MET:HE2	1.98	0.46
1:C:429:MET:HE3	1:C:438:PRO:HB2	1.98	0.46
1:E:123:TYR:OH	1:E:823:ARG:HD3	2.15	0.46
1:E:791:GLU:CD	1:E:861:ARG:HE	2.24	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:807:ILE:HG12	1:A:837:LEU:CD2	2.46	0.45
1:A:1032:GLU:OE1	1:A:1034:GLU:OE2	2.34	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:D:423:ASN:HD22	1:D:423:ASN:C	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:337:ILE:HG22	1:A:338:ALA:N	2.31	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:346:PHE:C	1:B:347:ILE:HD12	2.42	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: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:228:MET:HE3	1:C:232:VAL:HG21	1.96	0.45
1:C:681:SER:HB3	1:C:684:GLU:CG	2.45	0.45
1:C:976:LYS:HZ3	1:C:1017:ASP:HB2	1.82	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: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
1:D:404:LEU:HD22	1:D:429:MET:HE2	1.97	0.45
1:E:156:PHE:HD1	1:E:159:MET:CE	2.24	0.45
1:E:641:LEU:HD22	1:E:645:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PHE:HD1	1:B:159:MET:CE	2.26	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:446:GLU:CD	1:E:468:LYS:HG3	2.42	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:A:156:PHE:HD1	1:A:159:MET:CE	2.27	0.45
1:C:642:SER:HB2	1:C:647:THR:HB	1.99	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:469:HIS:HD1	1:A:473:ASP:CG	2.25	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:703:ASN:C	1:F:703:ASN:HD22	2.25	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: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:C:738:MET:SD	1:C:738:MET:C	3.00	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:B:568:LEU:HB3	1:B:571:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:ARG:HH22	1:A:216:GLU:CD	2.26	0.44
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:E:982:LEU:C	1:E:983:ILE:HD12	2.41	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:F:694:TRP:HA	1:F:738:MET:HE2	1.95	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:119:LYS:HZ1	1:B:823:ARG:HH22	1.64	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:C:423:ASN:C	1:C:423:ASN:ND2	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:771:LEU:C	1:E:771:LEU:HD13	2.43	0.44
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: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: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:514:TYR:CZ	1:E:540:PHE:HB2	2.53	0.44
1:B:203:LYS:HD3	1:B:740:GLY:C	2.42	0.43
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:124:PHE:O	1:C:125:SER:C	2.59	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:929:MET:HA	1:A:929:MET:CE	2.47	0.43
1:A:1031:VAL:CG1	1:A:1033:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:349:ASP:OD2	1:E:351:SER:OG	2.35	0.43
1:E:363:ARG:HG3	1:E:688:GLN:NE2	2.33	0.43
1:F:423:ASN:C	1:F:423:ASN:ND2	2.73	0.43
1:F:976:LYS:HZ3	1:F:1017:ASP:HB2	1.83	0.43
1:A:467:LEU:C	1:A:467:LEU:HD12	2.43	0.43
1:B:82:ASN:HD21	1:B:96:ARG:HD3	1.84	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: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:E:929:MET:HE3	1:E:979:LEU:CD1	2.48	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:929:MET:HA	1:E:929:MET:CE	2.46	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:A:887:MET:HE3	1:A:970:PHE:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:124:PHE:CE2	1:F:153:MET:HE1	2.53	0.43
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:703:ASN:C	1:A:703:ASN:ND2	2.75	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:155:PRO:HD2	1:D:159:MET:HE1	1.99	0.43
1:D:157:SER:HB3	1:D:856:ARG:NH1	2.34	0.43
1:D:241:ARG:HH12	1:D:263:ASP:CG	2.26	0.43
1:E:351:SER:HG	1:E:353:THR:HG22	1.82	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:A:190:ARG:NH2	1:A:216:GLU:CD	2.77	0.43
1:B:190:ARG:NH2	1:B:216:GLU:CD	2.76	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:403:ASN:ND2	1:E:403:ASN:C	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:141:ASP:OD2	1:A:141:ASP:C	2.62	0.43
1:A:373:THR:HA	1:A:392:TYR:CZ	2.54	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
1:C:771:LEU:HD13	1:C:771:LEU:C	2.43	0.43
1:D:428:ILE:HG23	1:D:441:ILE:HB	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:469:HIS:HD1	1:B:473:ASP:CG	2.27	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:F:886:ASP:OD2	1:F:886:ASP:C	2.61	0.42
1:A:889:MET:HE2	1:A:889:MET:HA	1.99	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: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: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:731:LEU:HD22	1:F:735:ILE:HG13	2.01	0.42
1:B:258:ASP:C	1:B:260:ASP:H	2.28	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: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:467:LEU:C	1:F:467:LEU:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:382:ARG:HD2	1:A:691:ASP:CG	2.45	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
1:E:886:ASP:OD2	1:E:886:ASP:C	2.62	0.42
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:568:LEU:HB3	1:A:571:MET:HE2	2.00	0.42
1:A:892:LEU:HD13	1:A:920:VAL:HG21	2.01	0.42
1:B:367:VAL:HG12	1:B:375:VAL:HG21	2.01	0.42
1:B:828:LYS:NZ	2:B:3341:HOH:O	2.40	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:258:ASP:C	1:D:260:ASP:H	2.26	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:F:154:GLN:HB3	1:F:159:MET:CE	2.42	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:159:MET:HE3	1:F:159:MET:HB2	1.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:929:MET:HE3	1:C:979:LEU:CG	2.49	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
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:C:664:LYS:C	1:C:666:GLU:H	2.27	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:828:LYS:NZ	2:F:7341:HOH:O	2.45	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:A:279:ASN:HD22	1:A:279:ASN:HA	1.78	0.41
1:B:289:LYS:NZ	2:B:3077:HOH:O	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:404:LEU:CD2	1:F:429:MET:HE1	2.50	0.41
1:A:428:ILE:HG23	1:A:441:ILE:HB	2.02	0.41
1:B:278:LEU:HD23	1:B:287:PHE:HB3	2.02	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:811:ASP:HB2	1:F:828:LYS:HE2	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:C:886:ASP:OD2	1:C:886:ASP:C	2.62	0.41
1:D:886:ASP:OD2	1:D:886:ASP:C	2.63	0.41
1:F:253:GLN:NE2	1:F:253:GLN:HA	2.35	0.41
1:F:662:LEU:HD23	1:F:662:LEU:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:811:ASP:O	1:B:811:ASP:CG	2.64	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: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: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:E:74:ILE:HG13	1:E:75:VAL:HG12	2.03	0.41
1:E:828:LYS:NZ	2:E:6341:HOH:O	2.44	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:A:241:ARG:HH12	1:A:263:ASP:CG	2.29	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:C:382:ARG:HD2	1:C:691:ASP:CG	2.46	0.41
1:C:929:MET:HE3	1:C:979:LEU:HD11	1.99	0.41
1:E:722:VAL:N	1:E:723:PRO:HD2	2.36	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: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:886:ASP:C	1:B:886:ASP:OD2	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:ILE:HG21	1:C:741:GLU:HG3	2.03	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:401:GLU:H	1:D:401:GLU:CD	2.28	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
1:F:242:ILE:O	1:F:256:SER:HA	2.21	0.41
1:F:326:ALA:C	1:F:327:GLU:HG3	2.45	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:F:771:LEU:HD13	1:F:771:LEU:C	2.46	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: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:429:MET:HE3	1:F:438:PRO:CB	2.50	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:241:ARG:HH12	1:B:263:ASP:CG	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:467:LEU:HD12	1:C:467:LEU:C	2.46	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: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:771:LEU:HD13	1:B:771:LEU:C	2.46	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:429:MET:HE3	1:C:438:PRO:CB	2.51	0.40
1:C:633:LYS:HE2	1:C:633:LYS:HB2	1.88	0.40
1:E:469:HIS:HD1	1:E:473:ASP:CG	2.28	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:628:LYS:HE3	2:E:6366:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:156:PHE:HD1	1:D:159:MET:CE	2.23	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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	30	27
1	B	1021/1045 (98%)	977 (96%)	41 (4%)	3 (0%)	37	35
1	C	1021/1045 (98%)	961 (94%)	53 (5%)	7 (1%)	19	14
1	D	1021/1045 (98%)	979 (96%)	38 (4%)	4 (0%)	30	27
1	E	1021/1045 (98%)	975 (96%)	43 (4%)	3 (0%)	37	35
1	F	1021/1045 (98%)	971 (95%)	44 (4%)	6 (1%)	22	17
All	All	6126/6270 (98%)	5842 (95%)	257 (4%)	27 (0%)	30	27

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ASP

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Mol	Chain	Res	Type
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
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%)	858 (97%)	25 (3%)	38	40
1	B	883/904 (98%)	857 (97%)	26 (3%)	37	39
1	C	883/904 (98%)	859 (97%)	24 (3%)	40	42
1	D	883/904 (98%)	854 (97%)	29 (3%)	33	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	883/904 (98%)	857 (97%)	26 (3%)	37 39
1	F	883/904 (98%)	859 (97%)	24 (3%)	40 42
All	All	5298/5424 (98%)	5144 (97%)	154 (3%)	37 39

All (154) 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	75	VAL
1	A	104	ASN
1	A	190	ARG
1	A	279	ASN
1	A	311	LEU
1	A	363	ARG
1	A	375	VAL
1	A	423	ASN
1	A	469	HIS
1	A	562	GLU
1	A	578	ILE
1	A	611	GLN
1	A	625	LYS
1	A	641	LEU
1	A	663	GLU
1	A	678	LEU
1	A	687	LEU
1	A	731	LEU
1	A	738	MET
1	A	892	LEU
1	A	929	MET
1	A	1024	ASN
1	B	44	LEU
1	B	61	LEU
1	B	75	VAL
1	B	104	ASN
1	B	114	GLU
1	B	190	ARG
1	B	279	ASN
1	B	311	LEU
1	B	313	SER

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Mol	Chain	Res	Type
1	B	330	SER
1	B	363	ARG
1	B	423	ASN
1	B	469	HIS
1	B	557	ARG
1	B	562	GLU
1	B	578	ILE
1	B	625	LYS
1	B	641	LEU
1	B	663	GLU
1	B	678	LEU
1	B	687	LEU
1	B	717	LYS
1	B	731	LEU
1	B	738	MET
1	B	892	LEU
1	B	929	MET
1	C	61	LEU
1	C	75	VAL
1	C	97	VAL
1	C	104	ASN
1	C	241	ARG
1	C	279	ASN
1	C	311	LEU
1	C	353	THR
1	C	363	ARG
1	C	403	ASN
1	C	423	ASN
1	C	469	HIS
1	C	557	ARG
1	C	562	GLU
1	C	578	ILE
1	C	625	LYS
1	C	641	LEU
1	C	663	GLU
1	C	687	LEU
1	C	731	LEU
1	C	738	MET
1	C	892	LEU
1	C	929	MET
1	C	1024	ASN
1	D	61	LEU

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Mol	Chain	Res	Type
1	D	75	VAL
1	D	82	ASN
1	D	97	VAL
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	429	MET
1	D	469	HIS
1	D	557	ARG
1	D	562	GLU
1	D	578	ILE
1	D	579	ASN
1	D	625	LYS
1	D	641	LEU
1	D	663	GLU
1	D	678	LEU
1	D	687	LEU
1	D	703	ASN
1	D	731	LEU
1	D	738	MET
1	D	892	LEU
1	D	1024	ASN
1	E	61	LEU
1	E	75	VAL
1	E	104	ASN
1	E	114	GLU
1	E	190	ARG
1	E	209	THR
1	E	218	ASN
1	E	241	ARG
1	E	311	LEU
1	E	363	ARG
1	E	403	ASN
1	E	423	ASN
1	E	429	MET
1	E	469	HIS

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Mol	Chain	Res	Type
1	E	557	ARG
1	E	562	GLU
1	E	578	ILE
1	E	579	ASN
1	E	625	LYS
1	E	641	LEU
1	E	663	GLU
1	E	731	LEU
1	E	738	MET
1	E	892	LEU
1	E	929	MET
1	E	1024	ASN
1	F	44	LEU
1	F	46	PRO
1	F	61	LEU
1	F	75	VAL
1	F	190	ARG
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	557	ARG
1	F	562	GLU
1	F	578	ILE
1	F	625	LYS
1	F	641	LEU
1	F	663	GLU
1	F	678	LEU
1	F	687	LEU
1	F	731	LEU
1	F	738	MET
1	F	892	LEU
1	F	929	MET
1	F	1024	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (201) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	64	HIS

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Mol	Chain	Res	Type
1	A	82	ASN
1	A	104	ASN
1	A	145	ASN
1	A	154	GLN
1	A	176	ASN
1	A	253	GLN
1	A	267	HIS
1	A	279	ASN
1	A	297	ASN
1	A	403	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
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	937	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	77	ASN
1	B	82	ASN
1	B	104	ASN
1	B	145	ASN
1	B	253	GLN
1	B	267	HIS
1	B	279	ASN
1	B	297	ASN

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Mol	Chain	Res	Type
1	B	403	ASN
1	B	423	ASN
1	B	481	HIS
1	B	497	ASN
1	B	499	HIS
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	937	ASN
1	B	949	ASN
1	B	1008	GLN
1	B	1024	ASN
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	145	ASN
1	C	171	ASN
1	C	176	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	499	HIS
1	C	511	ASN
1	C	530	ASN
1	C	579	ASN
1	C	611	GLN
1	C	635	ASN

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Mol	Chain	Res	Type
1	C	703	ASN
1	C	720	ASN
1	C	733	ASN
1	C	739	GLN
1	C	775	HIS
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	64	HIS
1	D	82	ASN
1	D	104	ASN
1	D	145	ASN
1	D	154	GLN
1	D	253	GLN
1	D	267	HIS
1	D	279	ASN
1	D	403	ASN
1	D	406	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

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Mol	Chain	Res	Type
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	64	HIS
1	E	82	ASN
1	E	104	ASN
1	E	145	ASN
1	E	154	GLN
1	E	195	ASN
1	E	253	GLN
1	E	267	HIS
1	E	279	ASN
1	E	403	ASN
1	E	406	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
1	E	635	ASN
1	E	688	GLN
1	E	720	ASN
1	E	733	ASN
1	E	739	GLN
1	E	867	ASN
1	E	872	HIS
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

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Mol	Chain	Res	Type
1	F	82	ASN
1	F	104	ASN
1	F	145	ASN
1	F	154	GLN
1	F	176	ASN
1	F	253	GLN
1	F	267	HIS
1	F	279	ASN
1	F	403	ASN
1	F	423	ASN
1	F	481	HIS
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
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 oligosaccharides 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, 95^{th} 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%)	0.49	56 (5%) 32 30	12, 26, 43, 56	19 (1%)
1	B	1022/1045 (97%)	0.49	62 (6%) 28 26	12, 26, 43, 55	19 (1%)
1	C	1022/1045 (97%)	0.98	113 (11%) 12 10	13, 32, 45, 56	19 (1%)
1	D	1022/1045 (97%)	0.63	73 (7%) 23 21	12, 28, 44, 54	19 (1%)
1	E	1022/1045 (97%)	0.58	62 (6%) 28 26	12, 28, 44, 55	19 (1%)
1	F	1022/1045 (97%)	0.92	110 (10%) 12 11	13, 32, 45, 55	19 (1%)
All	All	6132/6270 (97%)	0.68	476 (7%) 20 19	12, 29, 44, 56	114 (1%)

All (476) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	220	GLY	8.6
1	E	218	ASN	8.2
1	D	220	GLY	8.1
1	D	218	ASN	7.6
1	B	218	ASN	7.0
1	E	219	SER	6.7
1	D	219	SER	6.5
1	D	299	ASP	6.0
1	A	841	GLY	5.9
1	B	563	ALA	5.1
1	F	563	ALA	4.9
1	B	167	ASN	4.9
1	D	469	HIS	4.8
1	B	469	HIS	4.7
1	A	328	ASP	4.6
1	B	328	ASP	4.6
1	A	219	SER	4.5
1	F	218	ASN	4.5
1	D	716	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	299	ASP	4.4
1	E	716	GLU	4.4
1	A	218	ASN	4.3
1	D	642	SER	4.3
1	A	562	GLU	4.3
1	E	469	HIS	4.2
1	C	116	GLY	4.2
1	C	220	GLY	4.2
1	B	841	GLY	4.1
1	C	218	ASN	4.1
1	E	842	GLY	4.0
1	B	562	GLU	4.0
1	B	219	SER	4.0
1	C	219	SER	3.9
1	A	469	HIS	3.9
1	F	436	GLY	3.9
1	F	219	SER	3.9
1	F	401	GLU	3.9
1	A	167	ASN	3.9
1	D	612	GLY	3.8
1	D	297	ASN	3.8
1	A	436	GLY	3.7
1	C	188	GLY	3.7
1	F	1060	ARG	3.7
1	A	842	GLY	3.6
1	C	202	TRP	3.6
1	C	238	VAL	3.6
1	E	642	SER	3.6
1	D	286	LEU	3.6
1	B	642	SER	3.6
1	E	114	GLU	3.6
1	C	1060	ARG	3.6
1	A	300	THR	3.5
1	F	300	THR	3.5
1	A	188	GLY	3.5
1	A	396	LYS	3.5
1	C	243	TYR	3.5
1	F	729	TYR	3.5
1	F	362	LEU	3.5
1	F	712	GLU	3.5
1	D	826	SER	3.4
1	C	236	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	628	LYS	3.4
1	F	393	ARG	3.4
1	B	396	LYS	3.4
1	F	220	GLY	3.4
1	C	494	THR	3.4
1	C	221	ALA	3.4
1	B	716	GLU	3.4
1	D	774	ASP	3.4
1	B	612	GLY	3.4
1	E	171	ASN	3.3
1	A	308	ILE	3.3
1	B	286	LEU	3.3
1	C	282	GLY	3.3
1	D	560	THR	3.3
1	F	286	LEU	3.3
1	F	469	HIS	3.3
1	F	138	ALA	3.3
1	D	563	ALA	3.3
1	A	494	THR	3.3
1	C	562	GLU	3.3
1	E	560	THR	3.3
1	C	563	ALA	3.2
1	E	563	ALA	3.2
1	D	842	GLY	3.2
1	F	612	GLY	3.2
1	D	434	GLU	3.2
1	E	301	GLU	3.2
1	F	706	VAL	3.2
1	A	286	LEU	3.2
1	C	752	GLY	3.2
1	B	110	PHE	3.2
1	C	774	ASP	3.2
1	F	232	VAL	3.1
1	D	638	ASP	3.1
1	D	841	GLY	3.1
1	F	564	GLY	3.1
1	C	469	HIS	3.1
1	A	299	ASP	3.1
1	F	494	THR	3.1
1	C	185	PHE	3.1
1	C	184	LEU	3.1
1	B	436	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	171	ASN	3.1
1	A	560	THR	3.1
1	A	400	PHE	3.1
1	F	400	PHE	3.1
1	D	239	GLY	3.1
1	C	729	TYR	3.1
1	B	643	ALA	3.1
1	E	1017	ASP	3.1
1	B	400	PHE	3.0
1	C	286	LEU	3.0
1	D	561	SER	3.0
1	E	826	SER	3.0
1	B	842	GLY	3.0
1	C	807	ILE	3.0
1	A	67	LYS	3.0
1	E	300	THR	3.0
1	C	217	VAL	3.0
1	C	487	GLY	3.0
1	A	612	GLY	3.0
1	C	841	GLY	3.0
1	A	563	ALA	3.0
1	C	712	GLU	3.0
1	C	800	ILE	2.9
1	F	260	ASP	2.9
1	F	561	SER	2.9
1	F	562	GLU	2.9
1	E	308	ILE	2.9
1	F	306	ILE	2.9
1	A	627	ARG	2.9
1	A	676	ARG	2.9
1	C	168	ASP	2.9
1	C	846	ASP	2.9
1	B	188	GLY	2.9
1	E	260	ASP	2.9
1	D	330	SER	2.9
1	B	494	THR	2.9
1	A	564	GLY	2.9
1	C	173	VAL	2.8
1	E	286	LEU	2.8
1	F	722	VAL	2.8
1	A	653	ASP	2.8
1	C	853	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	643	ALA	2.8
1	D	171	ASN	2.8
1	C	988	TRP	2.8
1	B	853	ASP	2.8
1	D	706	VAL	2.8
1	E	329	PHE	2.8
1	D	548	SER	2.8
1	B	327	GLU	2.8
1	A	628	LYS	2.8
1	C	299	ASP	2.8
1	A	327	GLU	2.8
1	E	398	GLU	2.8
1	C	237	ILE	2.8
1	E	337	ILE	2.8
1	F	487	GLY	2.8
1	F	774	ASP	2.8
1	E	369	ARG	2.8
1	D	114	GLU	2.8
1	E	565	GLU	2.8
1	B	705	ALA	2.7
1	E	127	LYS	2.7
1	D	329	PHE	2.7
1	D	363	ARG	2.7
1	F	243	TYR	2.7
1	F	262	LYS	2.7
1	D	221	ALA	2.7
1	D	613	ALA	2.7
1	A	110	PHE	2.7
1	E	400	PHE	2.7
1	D	436	GLY	2.7
1	E	774	ASP	2.7
1	B	488	ARG	2.7
1	B	299	ASP	2.7
1	A	565	GLU	2.7
1	F	716	GLU	2.7
1	F	374	LYS	2.7
1	C	279	ASN	2.7
1	C	817	ALA	2.7
1	C	69	GLY	2.7
1	E	309	GLY	2.7
1	F	839	GLY	2.7
1	D	709	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	817	ALA	2.6
1	F	740	GLY	2.6
1	F	231	HIS	2.6
1	A	716	GLU	2.6
1	D	300	THR	2.6
1	E	471	GLU	2.6
1	C	142	PRO	2.6
1	D	641	LEU	2.6
1	A	488	ARG	2.6
1	B	217	VAL	2.6
1	C	706	VAL	2.6
1	F	238	VAL	2.6
1	F	252	GLY	2.6
1	F	402	GLU	2.6
1	B	774	ASP	2.6
1	F	270	PHE	2.6
1	F	853	ASP	2.6
1	D	308	ILE	2.6
1	F	297	ASN	2.6
1	E	330	SER	2.6
1	F	43	LEU	2.6
1	D	1017	ASP	2.6
1	B	319	ILE	2.6
1	E	676	ARG	2.6
1	A	433	LEU	2.6
1	C	489	LYS	2.5
1	C	165	VAL	2.5
1	B	300	THR	2.5
1	B	560	THR	2.5
1	C	110	PHE	2.5
1	D	425	ARG	2.5
1	F	761	ARG	2.5
1	C	144	GLY	2.5
1	E	612	GLY	2.5
1	F	628	LYS	2.5
1	A	705	ALA	2.5
1	A	1017	ASP	2.5
1	D	935	TYR	2.5
1	E	91	ARG	2.5
1	C	171	ASN	2.5
1	E	937	ASN	2.5
1	A	319	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1033	ILE	2.5
1	C	1056	ILE	2.5
1	A	1058	GLU	2.5
1	D	402	GLU	2.5
1	D	565	GLU	2.5
1	C	50	GLY	2.5
1	C	397	ALA	2.5
1	A	557	ARG	2.5
1	B	445	ARG	2.5
1	D	435	THR	2.5
1	E	706	VAL	2.5
1	C	45	ASN	2.5
1	C	112	ASN	2.5
1	C	114	GLU	2.5
1	B	561	SER	2.5
1	D	944	SER	2.5
1	B	91	ARG	2.5
1	F	627	ARG	2.5
1	D	705	ALA	2.5
1	C	300	THR	2.5
1	D	626	THR	2.5
1	B	434	GLU	2.4
1	C	401	GLU	2.4
1	A	839	GLY	2.4
1	D	1019	GLY	2.4
1	E	395	GLY	2.4
1	B	772	ASP	2.4
1	C	89	ASP	2.4
1	E	627	ARG	2.4
1	F	723	PRO	2.4
1	F	273	TYR	2.4
1	F	248	ILE	2.4
1	F	983	ILE	2.4
1	C	113	GLY	2.4
1	D	369	ARG	2.4
1	F	69	GLY	2.4
1	A	774	ASP	2.4
1	C	258	ASP	2.4
1	F	59	ASP	2.4
1	F	272	ASP	2.4
1	C	1031	VAL	2.4
1	E	840	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	736	VAL	2.4
1	C	88	PRO	2.4
1	A	393	ARG	2.4
1	C	445	ARG	2.4
1	C	627	ARG	2.4
1	C	1011	PHE	2.4
1	C	334	GLY	2.4
1	D	371	GLY	2.4
1	F	841	GLY	2.4
1	C	402	GLU	2.4
1	E	434	GLU	2.4
1	C	186	ALA	2.4
1	D	646	LYS	2.4
1	C	298	PRO	2.4
1	C	549	PRO	2.4
1	E	561	SER	2.4
1	B	393	ARG	2.4
1	C	329	PHE	2.4
1	D	1020	PHE	2.4
1	E	564	GLY	2.4
1	F	1017	ASP	2.4
1	F	170	ILE	2.4
1	C	327	GLU	2.3
1	C	259	LEU	2.3
1	C	82	ASN	2.3
1	D	374	LYS	2.3
1	C	779	ALA	2.3
1	F	152	ALA	2.3
1	B	435	THR	2.3
1	A	706	VAL	2.3
1	B	629	VAL	2.3
1	B	706	VAL	2.3
1	D	557	ARG	2.3
1	A	772	ASP	2.3
1	D	843	ASP	2.3
1	E	846	ASP	2.3
1	A	339	PHE	2.3
1	F	329	PHE	2.3
1	C	306	ILE	2.3
1	F	237	ILE	2.3
1	F	308	ILE	2.3
1	A	641	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	840	LYS	2.3
1	E	417	LYS	2.3
1	F	840	LYS	2.3
1	E	221	ALA	2.3
1	E	548	SER	2.3
1	A	217	VAL	2.3
1	D	629	VAL	2.3
1	D	335	ASP	2.3
1	E	370	GLY	2.3
1	F	51	ASP	2.3
1	F	188	GLY	2.3
1	C	337	ILE	2.3
1	D	905	TYR	2.3
1	F	255	TYR	2.3
1	F	557	ARG	2.3
1	F	676	ARG	2.3
1	C	642	SER	2.3
1	B	1017	ASP	2.3
1	B	1058	GLU	2.3
1	F	1015	PHE	2.3
1	F	64	HIS	2.3
1	A	807	ILE	2.3
1	C	242	ILE	2.3
1	B	676	ARG	2.3
1	D	382	ARG	2.3
1	C	724	LEU	2.3
1	E	641	LEU	2.3
1	F	153	MET	2.3
1	A	435	THR	2.3
1	B	397	ALA	2.3
1	C	613	ALA	2.3
1	D	643	ALA	2.3
1	F	397	ALA	2.3
1	F	440	VAL	2.2
1	F	992	VAL	2.2
1	C	262	LYS	2.2
1	C	628	LYS	2.2
1	F	266	LYS	2.2
1	D	415	ASN	2.2
1	A	329	PHE	2.2
1	C	1015	PHE	2.2
1	B	39	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	433	LEU	2.2
1	F	771	LEU	2.2
1	F	105	THR	2.2
1	C	166	GLU	2.2
1	A	561	SER	2.2
1	F	438	PRO	2.2
1	F	310	ASP	2.2
1	C	740	GLY	2.2
1	E	239	GLY	2.2
1	E	334	GLY	2.2
1	E	841	GLY	2.2
1	F	891	GLY	2.2
1	F	236	VAL	2.2
1	B	640	ARG	2.2
1	C	415	ASN	2.2
1	F	185	PHE	2.2
1	B	308	ILE	2.2
1	D	542	ILE	2.2
1	F	293	ILE	2.2
1	B	663	GLU	2.2
1	C	301	GLU	2.2
1	D	494	THR	2.2
1	C	843	ASP	2.2
1	F	399	LYS	2.2
1	B	370	GLY	2.2
1	C	91	ARG	2.2
1	D	937	ASN	2.2
1	F	1011	PHE	2.2
1	A	1034	GLU	2.2
1	C	303	ILE	2.2
1	D	562	GLU	2.2
1	C	66	LEU	2.2
1	F	390	TYR	2.2
1	C	288	SER	2.2
1	C	260	ASP	2.2
1	E	328	ASP	2.2
1	A	445	ARG	2.2
1	D	188	GLY	2.2
1	D	470	GLY	2.2
1	C	375	VAL	2.2
1	E	992	VAL	2.2
1	F	97	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	649	MET	2.2
1	B	329	PHE	2.1
1	C	662	LEU	2.1
1	C	983	ILE	2.1
1	F	54	ILE	2.1
1	B	844	LYS	2.1
1	C	844	LYS	2.1
1	D	489	LYS	2.1
1	F	305	LYS	2.1
1	B	653	ASP	2.1
1	B	843	ASP	2.1
1	A	91	ARG	2.1
1	C	111	TYR	2.1
1	D	488	ARG	2.1
1	F	445	ARG	2.1
1	C	665	PRO	2.1
1	C	839	GLY	2.1
1	F	842	GLY	2.1
1	F	624	VAL	2.1
1	B	800	ILE	2.1
1	B	807	ILE	2.1
1	C	969	ILE	2.1
1	F	807	ILE	2.1
1	C	670	THR	2.1
1	D	1060	ARG	2.1
1	F	187	ASP	2.1
1	F	247	ASP	2.1
1	F	643	ALA	2.1
1	A	40	PRO	2.1
1	C	297	ASN	2.1
1	D	569	ASN	2.1
1	E	649	MET	2.1
1	D	217	VAL	2.1
1	B	557	ARG	2.1
1	B	627	ARG	2.1
1	E	657	ILE	2.1
1	E	687	LEU	2.1
1	F	335	ASP	2.1
1	F	435	THR	2.1
1	F	800	ILE	2.1
1	E	643	ALA	2.1
1	F	705	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	487	GLY	2.1
1	B	665	PRO	2.1
1	C	179	PRO	2.1
1	F	371	GLY	2.1
1	C	1040	TYR	2.1
1	F	396	LYS	2.1
1	C	51	ASP	2.1
1	E	1053	ASP	2.1
1	F	65	ASP	2.1
1	C	837	LEU	2.1
1	F	826	SER	2.1
1	F	471	GLU	2.0
1	C	255	TYR	2.0
1	C	187	ASP	2.0
1	D	581	ASP	2.0
1	F	299	ASP	2.0
1	E	944	SER	2.0
1	D	271	THR	2.0
1	D	995	THR	2.0
1	C	197	PHE	2.0
1	C	400	PHE	2.0
1	E	170	ILE	2.0
1	F	110	PHE	2.0
1	B	1034	GLU	2.0
1	D	334	GLY	2.0
1	E	592	GLU	2.0
1	F	166	GLU	2.0
1	F	304	GLU	2.0
1	E	297	ASN	2.0
1	F	613	ALA	2.0
1	A	437	LYS	2.0
1	A	761	ARG	2.0
1	B	489	LYS	2.0
1	C	363	ARG	2.0
1	E	294	TYR	2.0
1	C	624	VAL	2.0
1	D	667	ASP	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.