



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:29 PM EDT

PDB ID : 3S51 / pdb_00003s51
Title : Structure of FANCI
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

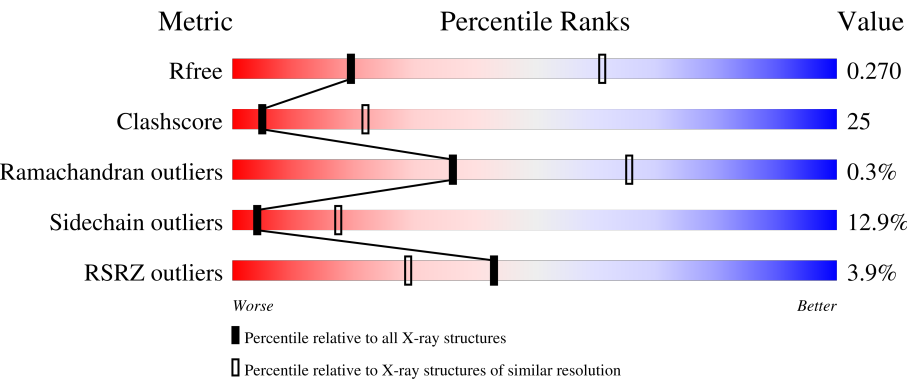
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	1308	5% 43%37%7%13%
1	B	1308	% 39%36%7%18%
1	C	1308	5% 43%37%6%13%
1	D	1308	2% 39%33%6%21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34594 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 Fanconi anemia group I protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	B	1071	Total	C	N	O	S	0	0	0
			8487	5468	1409	1559	51			
1	C	1134	Total	C	N	O	S	0	0	0
			8960	5762	1489	1656	53			
1	D	1034	Total	C	N	O	S	0	0	0
			8187	5277	1358	1504	48			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	expression tag	UNP Q8K368
A	1304	HIS	-	expression tag	UNP Q8K368
A	1305	HIS	-	expression tag	UNP Q8K368
A	1306	HIS	-	expression tag	UNP Q8K368
A	1307	HIS	-	expression tag	UNP Q8K368
A	1308	HIS	-	expression tag	UNP Q8K368
B	1303	HIS	-	expression tag	UNP Q8K368
B	1304	HIS	-	expression tag	UNP Q8K368
B	1305	HIS	-	expression tag	UNP Q8K368
B	1306	HIS	-	expression tag	UNP Q8K368
B	1307	HIS	-	expression tag	UNP Q8K368
B	1308	HIS	-	expression tag	UNP Q8K368
C	1303	HIS	-	expression tag	UNP Q8K368
C	1304	HIS	-	expression tag	UNP Q8K368
C	1305	HIS	-	expression tag	UNP Q8K368
C	1306	HIS	-	expression tag	UNP Q8K368
C	1307	HIS	-	expression tag	UNP Q8K368
C	1308	HIS	-	expression tag	UNP Q8K368
D	1303	HIS	-	expression tag	UNP Q8K368
D	1304	HIS	-	expression tag	UNP Q8K368
D	1305	HIS	-	expression tag	UNP Q8K368

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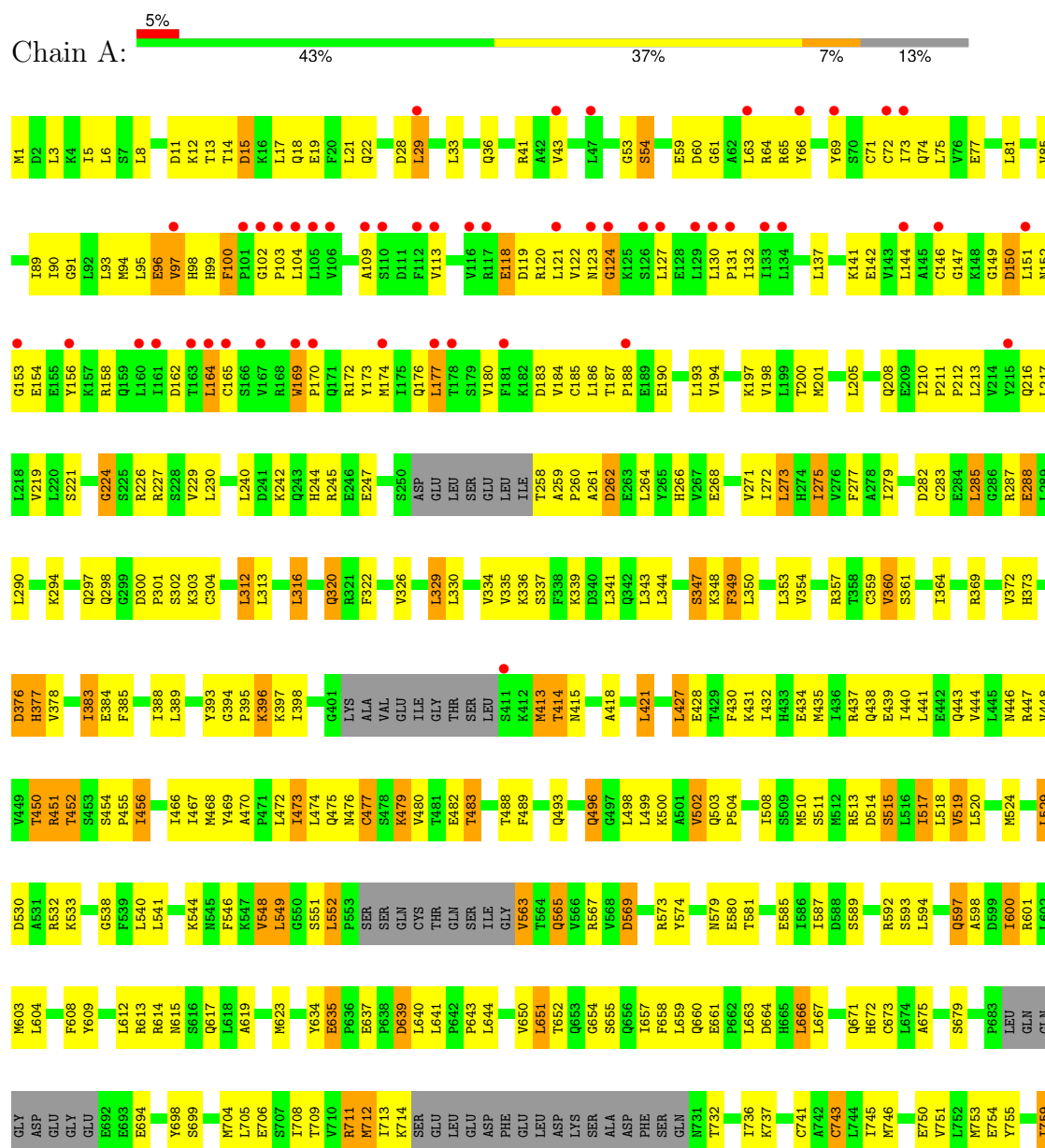
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1306	HIS	-	expression tag	UNP Q8K368
D	1307	HIS	-	expression tag	UNP Q8K368
D	1308	HIS	-	expression tag	UNP Q8K368

3 Residue-property plots

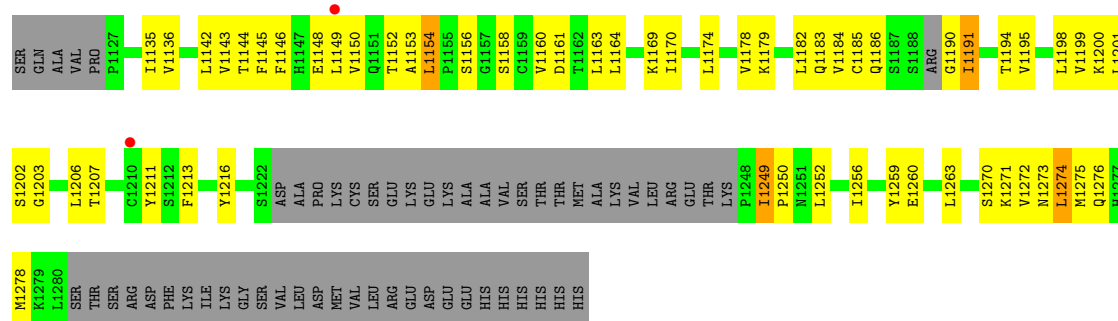
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fanconi anemia group I protein homolog

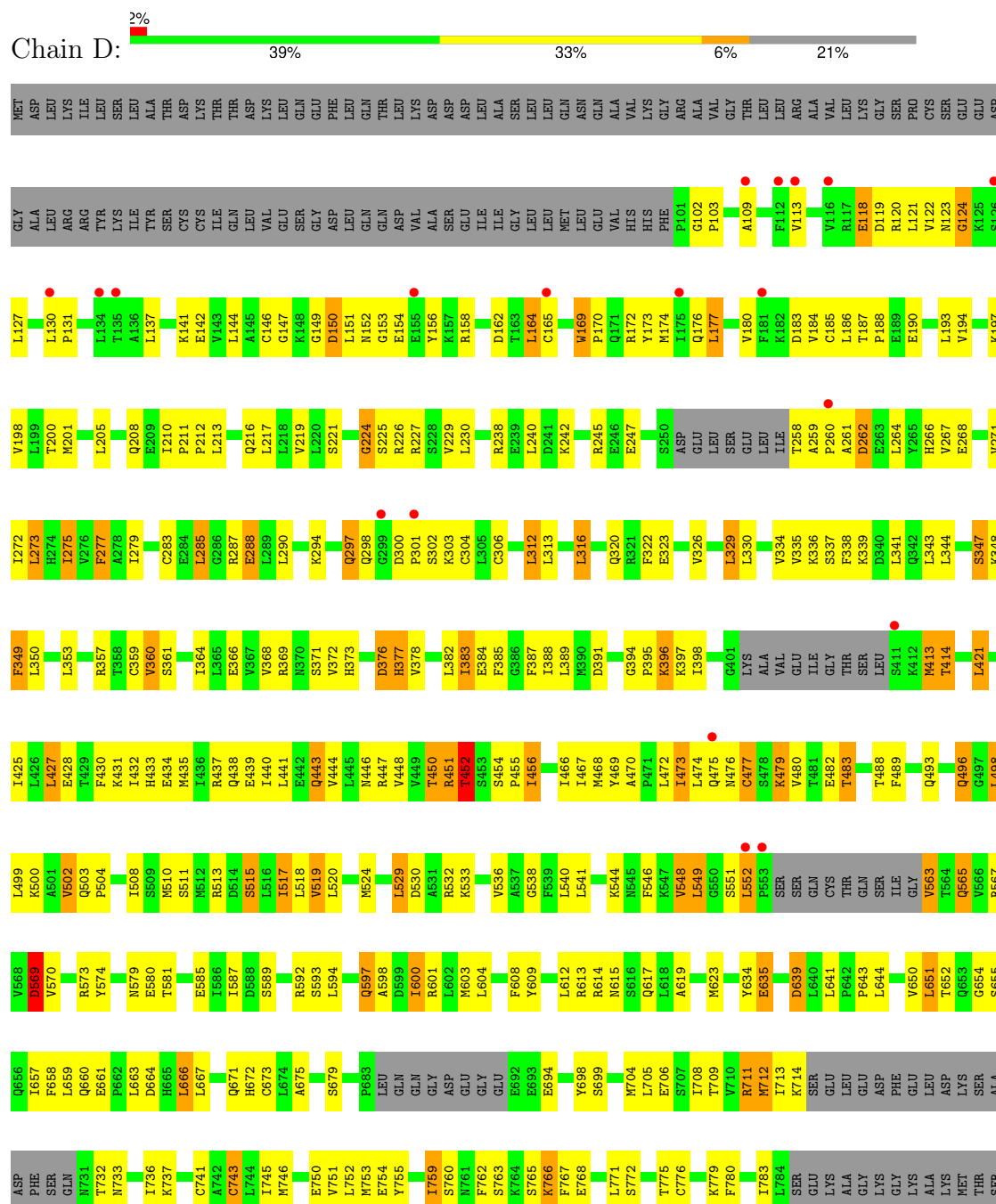








• Molecule 1: Fanconi anemia group I protein homolog



E1260	Q1186	THR	Q949	R878	K798
L1263	S1187	LEU	R950	V879	V799
S1270	S1188	SER	A951	L880	S800
K1271	S1189	ASP	S952	L881	S801
V1272	G1190	LYS	F953	W882	S802
M1273	I1191	VAL	Q954	T885	L803
L1274	T1194	THR	Q957	S886	L804
M1275	V1195	PRO	F958	I1E	S805
Q1276	L1198	GLU	Q959	THR	L806
H1277	V1199	ASP	R960	L812	L813
M1278	K1200	ALA	L965	SER	T814
K1279	L1201	SER	L966	VAL	A815
L1280	S1202	GLN	F973	GLU	A816
THR	G1203	VAL	N974	SER	F817
SER	P1127	PRO	S975	GLY	R818
ARG	L1206	ASP	K976	LYS	D819
ASP	T1207	GLN	E977	LYS	H824
PHE	Y1211	ASP	A978	GLU	E825
LYS	Y1216	VAL	L979	LYS	E826
ILE	Y1217	GLU	L980	GLY	S827
GLY	S1222	ILE	L981	LYS	L828
SER	ASP	GLU	I982	LYS	S829
VAL	ALA	LYS	L985	VAL	V830
LEU	PRO	THR	L988	L831	L832
GLU	LYS	ASP	L989	S833	S834
ASP	PRO	PHE	S997	G835	G836
MET	LYS	ALA	L992	F837	M838
VAL	CYS	VAL	E993	H839	N843
LEU	SER	V1150	P994	T914	L846
ARG	GLU	Q1151	T995	F915	Q847
GLU	LYS	A1076	S996	V918	K848
GLU	LYS	A1077	P997	L919	L852
GLU	ALA	P1078	Q998	Y922	L853
ALA	ALA	T1079	F999	Q923	V858
VAL	VAL	V1080	V1000	P924	S859
SER	THR	L1083	Q1001	L930	G860
THR	THR	V1084	M1002	F929	P861
MET	ALA	L1085	L1003	Q931	T862
LYS	LYS	S1086	W1005	D934	G863
VAL	VAL	Q1087	I1009	VAL	Q864
LEU	LEU	K1090	Y1013	MET	N865
ARG	ARG	V1091	S1014	GLY	L869
GLU	GLU	L1092	Q1015	THR	F870
THR	THR	E1093	S1019	GLU	Q871
LYS	LYS	V1094	K1022	GLU	N872
P1248	V1178	V1095	ALA	ALA	T877
I1249	K1179	K1103	S1023	GLY	
P1250	G1180	S1105	L1024	V945	
N1251	Y1181	H1106	M1025	V947	
L1252	L1182	ASN	F1029	T948	
Y1256	Q1183	GLN			
Y1259	V1184	GLU			
	C1185				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	114.70Å 136.50Å 149.70Å 115.90° 106.00° 95.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	82.8 (39.82-3.30) 84.5 (39.82-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.259 , 0.278 0.246 , 0.270	Depositor DCC
R_{free} test set	2199 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 139.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34594	wwPDB-VP
Average B, all atoms (Å ²)	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.34	2/9099 (0.0%)	0.80	15/12286 (0.1%)
1	B	0.36	4/8624 (0.0%)	0.80	13/11646 (0.1%)
1	C	0.34	2/9099 (0.0%)	0.80	12/12286 (0.1%)
1	D	0.33	2/8319 (0.0%)	0.80	12/11234 (0.1%)
All	All	0.34	10/35141 (0.0%)	0.80	52/47452 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	959	GLN	CD-NE2	-12.08	1.07	1.33
1	B	959	GLN	CD-OE1	-8.82	1.06	1.23
1	C	320	GLN	CD-NE2	-8.24	1.16	1.33
1	D	320	GLN	CD-NE2	-8.04	1.16	1.33
1	A	320	GLN	CD-NE2	-7.51	1.17	1.33
1	B	320	GLN	CD-NE2	-7.50	1.17	1.33
1	D	320	GLN	CD-OE1	-6.91	1.10	1.23
1	C	320	GLN	CD-OE1	-6.81	1.10	1.23
1	A	320	GLN	CD-OE1	-6.80	1.10	1.23
1	B	320	GLN	CD-OE1	-6.74	1.10	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	GLY	N-CA-C	8.57	123.62	112.13
1	D	224	GLY	N-CA-C	8.56	123.60	112.13
1	B	224	GLY	N-CA-C	8.51	123.54	112.13
1	A	224	GLY	N-CA-C	8.39	123.37	112.13
1	C	1037	SER	CA-C-N	8.25	127.91	119.82
1	C	1037	SER	C-N-CA	8.25	127.91	119.82
1	A	1037	SER	CA-C-N	8.16	127.81	119.82
1	A	1037	SER	C-N-CA	8.16	127.81	119.82
1	D	1037	SER	CA-C-N	8.14	127.80	119.82
1	D	1037	SER	C-N-CA	8.14	127.80	119.82
1	B	1037	SER	CA-C-N	8.11	127.77	119.82
1	B	1037	SER	C-N-CA	8.11	127.77	119.82
1	B	860	GLY	CA-C-N	7.87	127.93	119.90
1	B	860	GLY	C-N-CA	7.87	127.93	119.90
1	D	860	GLY	CA-C-N	7.78	127.83	119.90
1	D	860	GLY	C-N-CA	7.78	127.83	119.90
1	A	860	GLY	CA-C-N	7.71	127.77	119.90
1	A	860	GLY	C-N-CA	7.71	127.77	119.90
1	C	860	GLY	CA-C-N	7.67	127.72	119.90
1	C	860	GLY	C-N-CA	7.67	127.72	119.90
1	A	100	PHE	CA-C-N	-7.59	112.87	120.31
1	A	100	PHE	C-N-CA	-7.59	112.87	120.31
1	C	28	ASP	N-CA-C	-6.77	104.64	113.17
1	A	28	ASP	N-CA-C	-6.72	104.70	113.17
1	D	635	GLU	CA-C-N	5.64	125.17	119.19
1	D	635	GLU	C-N-CA	5.64	125.17	119.19
1	B	635	GLU	CA-C-N	5.63	125.16	119.19
1	B	635	GLU	C-N-CA	5.63	125.16	119.19
1	B	959	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	C	635	GLU	CA-C-N	5.58	125.11	119.19
1	C	635	GLU	C-N-CA	5.58	125.11	119.19
1	D	546	PHE	N-CA-C	5.46	117.99	108.76
1	B	546	PHE	N-CA-C	5.43	117.93	108.76
1	A	635	GLU	CA-C-N	5.42	124.94	119.19
1	A	635	GLU	C-N-CA	5.42	124.94	119.19
1	C	1191	ILE	CA-C-N	5.40	125.70	119.92
1	C	1191	ILE	C-N-CA	5.40	125.70	119.92
1	A	1191	ILE	CA-C-N	5.40	125.70	119.92
1	A	1191	ILE	C-N-CA	5.40	125.70	119.92
1	B	1191	ILE	CA-C-N	5.40	125.70	119.92
1	B	1191	ILE	C-N-CA	5.40	125.70	119.92
1	D	1191	ILE	CA-C-N	5.28	125.57	119.92
1	D	1191	ILE	C-N-CA	5.28	125.57	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	546	PHE	N-CA-C	5.20	117.89	108.69
1	A	124	GLY	N-CA-C	-5.18	107.57	115.66
1	B	124	GLY	N-CA-C	-5.17	107.60	115.66
1	C	124	GLY	N-CA-C	-5.17	107.60	115.66
1	A	546	PHE	N-CA-C	5.15	117.81	108.69
1	D	569	ASP	N-CA-C	5.08	118.64	112.23
1	A	354	VAL	N-CA-C	5.03	113.47	107.73
1	D	124	GLY	N-CA-C	-5.03	107.81	115.66
1	B	354	VAL	N-CA-C	5.03	113.46	107.73

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	LEU	Peptide
1	B	1053	LEU	Peptide
1	C	1053	LEU	Peptide
1	D	1053	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8960	0	9275	469	0
1	B	8487	0	8776	469	0
1	C	8960	0	9275	454	0
1	D	8187	0	8476	429	0
All	All	34594	0	35802	1771	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 25.

All (1771) 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:C:799:VAL:O	1:C:847:GLN:NE2	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:VAL:O	1:A:847:GLN:NE2	1.88	1.07
1:B:799:VAL:O	1:B:847:GLN:NE2	1.88	1.06
1:D:799:VAL:O	1:D:847:GLN:NE2	1.88	1.05
1:A:489:PHE:HB3	1:C:450:THR:HG21	1.35	1.04
1:A:450:THR:HG21	1:C:489:PHE:HB3	1.38	1.01
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.43	1.01
1:B:77:GLU:HB2	1:B:121:LEU:HA	1.43	1.00
1:D:259:ALA:HB3	1:D:260:PRO:HD3	1.44	0.99
1:C:259:ALA:HB3	1:C:260:PRO:HD3	1.43	0.99
1:B:259:ALA:HB3	1:B:260:PRO:HD3	1.43	0.97
1:A:376:ASP:HB2	1:B:570:VAL:HG21	1.45	0.96
1:B:672:HIS:ND1	1:B:861:PRO:HG3	1.83	0.94
1:B:94:MET:HA	1:B:129:LEU:HD21	1.48	0.93
1:A:671:GLN:HE21	1:A:755:TYR:HA	1.35	0.92
1:D:713:ILE:O	1:D:714:LYS:HG2	1.71	0.91
1:C:713:ILE:O	1:C:714:LYS:HG2	1.70	0.91
1:B:713:ILE:O	1:B:714:LYS:HG2	1.72	0.90
1:A:1055:ASP:H	1:A:1152:THR:HA	1.36	0.90
1:A:713:ILE:O	1:A:714:LYS:HG2	1.71	0.89
1:A:335:VAL:HG13	1:A:414:THR:HG21	1.54	0.89
1:A:29:LEU:O	1:A:33:LEU:HG	1.73	0.86
1:D:672:HIS:ND1	1:D:861:PRO:HG3	1.90	0.86
1:C:29:LEU:O	1:C:33:LEU:HG	1.74	0.86
1:B:452:THR:HA	1:D:452:THR:HA	1.58	0.85
1:C:598:ALA:HB2	1:C:660:GLN:HA	1.59	0.85
1:A:94:MET:HE3	1:A:132:ILE:HD11	1.59	0.85
1:A:598:ALA:HB2	1:A:660:GLN:HA	1.59	0.85
1:A:641:LEU:O	1:A:643:PRO:HD3	1.78	0.84
1:B:1055:ASP:H	1:B:1152:THR:HA	1.43	0.83
1:B:598:ALA:HB2	1:B:660:GLN:HA	1.59	0.83
1:B:77:GLU:OE1	1:B:121:LEU:HD23	1.78	0.83
1:B:816:LEU:HD13	1:B:838:MET:HE1	1.61	0.83
1:C:1055:ASP:H	1:C:1152:THR:HA	1.42	0.83
1:B:100:PHE:HD2	1:B:104:LEU:HB3	1.43	0.83
1:B:301:PRO:HA	1:B:304:CYS:HB2	1.60	0.83
1:D:1077:ALA:HB3	1:D:1078:PRO:HD3	1.61	0.83
1:C:1077:ALA:HB3	1:C:1078:PRO:HD3	1.61	0.83
1:C:301:PRO:HA	1:C:304:CYS:HB2	1.60	0.83
1:A:1077:ALA:HB3	1:A:1078:PRO:HD3	1.61	0.83
1:B:227:ARG:HG3	1:B:288:GLU:HG3	1.61	0.83
1:A:301:PRO:HA	1:A:304:CYS:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:ALA:HB2	1:D:660:GLN:HA	1.59	0.82
1:C:641:LEU:O	1:C:643:PRO:HD3	1.78	0.82
1:D:816:LEU:HD13	1:D:838:MET:HE1	1.61	0.82
1:A:672:HIS:ND1	1:A:861:PRO:HG3	1.95	0.81
1:B:258:THR:N	1:B:261:ALA:HB3	1.95	0.81
1:D:1055:ASP:H	1:D:1152:THR:HA	1.45	0.81
1:A:258:THR:N	1:A:261:ALA:HB3	1.95	0.81
1:B:1077:ALA:HB3	1:B:1078:PRO:HD3	1.61	0.81
1:B:641:LEU:O	1:B:643:PRO:HD3	1.79	0.81
1:B:450:THR:HG21	1:D:489:PHE:HB3	1.63	0.81
1:D:301:PRO:HA	1:D:304:CYS:HB2	1.60	0.81
1:D:641:LEU:O	1:D:643:PRO:HD3	1.80	0.81
1:D:258:THR:N	1:D:261:ALA:HB3	1.96	0.80
1:C:816:LEU:HD13	1:C:838:MET:HE1	1.62	0.80
1:C:1056:ILE:HG12	1:C:1153:ALA:HB2	1.64	0.80
1:A:816:LEU:HD13	1:A:838:MET:HE1	1.63	0.80
1:D:217:LEU:HD22	1:D:229:VAL:HG13	1.64	0.80
1:C:258:THR:N	1:C:261:ALA:HB3	1.96	0.79
1:C:217:LEU:HD22	1:C:229:VAL:HG13	1.63	0.79
1:B:623:MET:HE1	1:B:673:CYS:HB3	1.64	0.79
1:C:65:ARG:HB3	1:C:100:PHE:HZ	1.48	0.79
1:C:623:MET:HE1	1:C:673:CYS:HB3	1.65	0.79
1:D:623:MET:HE1	1:D:673:CYS:HB3	1.64	0.78
1:A:217:LEU:HD22	1:A:229:VAL:HG13	1.63	0.78
1:A:623:MET:HE1	1:A:673:CYS:HB3	1.64	0.78
1:C:427:LEU:HD22	1:C:431:LYS:HD2	1.65	0.78
1:A:302:SER:HB2	1:A:357:ARG:HG2	1.66	0.78
1:A:65:ARG:HB3	1:A:100:PHE:HZ	1.47	0.78
1:B:302:SER:HB2	1:B:357:ARG:HG2	1.66	0.78
1:D:302:SER:HB2	1:D:357:ARG:HG2	1.66	0.78
1:B:165:CYS:HB3	1:B:197:LYS:HG3	1.66	0.77
1:A:1054:GLY:HA3	1:A:1153:ALA:H	1.48	0.77
1:B:217:LEU:HD22	1:B:229:VAL:HG13	1.65	0.77
1:A:452:THR:HA	1:C:452:THR:HA	1.67	0.77
1:D:371:SER:OG	1:D:433:HIS:CE1	2.38	0.77
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.66	0.77
1:C:302:SER:HB2	1:C:357:ARG:HG2	1.66	0.77
1:C:671:GLN:HE21	1:C:755:TYR:HA	1.50	0.77
1:B:489:PHE:HB3	1:D:450:THR:HG21	1.66	0.77
1:C:349:PHE:H	1:C:349:PHE:HD2	1.33	0.77
1:B:1056:ILE:HG12	1:B:1153:ALA:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ALA:O	1:A:473:ILE:HG13	1.86	0.76
1:C:470:ALA:O	1:C:473:ILE:HG13	1.86	0.76
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.67	0.76
1:D:377:HIS:CD2	1:D:377:HIS:H	2.05	0.75
1:B:65:ARG:HB3	1:B:100:PHE:HZ	1.51	0.75
1:B:149:GLY:O	1:B:151:LEU:N	2.19	0.75
1:C:377:HIS:H	1:C:377:HIS:CD2	2.04	0.75
1:B:470:ALA:O	1:B:473:ILE:HG13	1.86	0.75
1:D:371:SER:OG	1:D:433:HIS:HE1	1.70	0.75
1:C:1054:GLY:O	1:C:1055:ASP:HB2	1.87	0.75
1:D:165:CYS:HB3	1:D:197:LYS:HG3	1.66	0.75
1:D:259:ALA:CB	1:D:260:PRO:HD3	2.17	0.75
1:B:377:HIS:H	1:B:377:HIS:CD2	2.05	0.75
1:C:259:ALA:CB	1:C:260:PRO:HD3	2.16	0.75
1:B:94:MET:HA	1:B:129:LEU:CD2	2.16	0.75
1:B:349:PHE:H	1:B:349:PHE:HD2	1.33	0.75
1:A:349:PHE:HD2	1:A:349:PHE:H	1.33	0.75
1:A:377:HIS:CD2	1:A:377:HIS:H	2.04	0.75
1:B:338:PHE:CD2	1:B:414:THR:HG23	2.22	0.74
1:D:1054:GLY:O	1:D:1055:ASP:HB2	1.87	0.74
1:B:259:ALA:CB	1:B:260:PRO:HD3	2.17	0.74
1:B:452:THR:HB	1:B:454:SER:H	1.51	0.74
1:D:427:LEU:HD22	1:D:431:LYS:HD2	1.69	0.74
1:D:452:THR:HB	1:D:454:SER:H	1.51	0.74
1:C:165:CYS:HB3	1:C:197:LYS:HG3	1.67	0.74
1:A:1054:GLY:O	1:A:1055:ASP:HB2	1.87	0.74
1:C:452:THR:HB	1:C:454:SER:H	1.51	0.74
1:D:470:ALA:O	1:D:473:ILE:HG13	1.87	0.74
1:D:1056:ILE:HG12	1:D:1153:ALA:HB2	1.68	0.74
1:B:1014:SER:HB3	1:B:1070:VAL:HG12	1.70	0.73
1:D:149:GLY:O	1:D:151:LEU:N	2.21	0.73
1:A:946:THR:O	1:A:950:ARG:HG2	1.88	0.73
1:A:1056:ILE:HG12	1:A:1153:ALA:HB2	1.70	0.73
1:A:1146:PHE:CD1	1:A:1170:ILE:HD11	2.23	0.73
1:B:474:LEU:O	1:B:477:CYS:HB2	1.89	0.73
1:A:149:GLY:O	1:A:151:LEU:N	2.20	0.73
1:B:1054:GLY:O	1:B:1055:ASP:HB2	1.87	0.73
1:B:1146:PHE:CD1	1:B:1170:ILE:HD11	2.23	0.73
1:B:1203:GLY:HA3	1:B:1278:MET:CG	2.19	0.73
1:A:452:THR:HB	1:A:454:SER:H	1.51	0.73
1:A:1014:SER:HB3	1:A:1070:VAL:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1146:PHE:CD1	1:C:1170:ILE:HD11	2.23	0.73
1:B:297:GLN:HG3	1:B:1104:GLY:HA2	1.71	0.73
1:C:94:MET:HE3	1:C:132:ILE:HD11	1.71	0.73
1:D:474:LEU:O	1:D:477:CYS:HB2	1.89	0.73
1:A:474:LEU:O	1:A:477:CYS:HB2	1.88	0.73
1:B:427:LEU:HD22	1:B:431:LYS:HD2	1.69	0.73
1:D:1014:SER:HB3	1:D:1070:VAL:HG12	1.70	0.73
1:B:946:THR:O	1:B:950:ARG:HG2	1.89	0.73
1:C:474:LEU:O	1:C:477:CYS:HB2	1.88	0.72
1:C:946:THR:O	1:C:950:ARG:HG2	1.88	0.72
1:A:548:VAL:O	1:A:549:LEU:HB3	1.89	0.72
1:D:1146:PHE:CD1	1:D:1170:ILE:HD11	2.23	0.72
1:B:297:GLN:HG3	1:B:1104:GLY:CA	2.19	0.72
1:D:349:PHE:H	1:D:349:PHE:HD2	1.33	0.72
1:C:1014:SER:HB3	1:C:1070:VAL:HG12	1.70	0.72
1:B:548:VAL:O	1:B:549:LEU:HB3	1.88	0.72
1:C:544:LYS:O	1:C:614:ARG:HD2	1.90	0.72
1:D:946:THR:O	1:D:950:ARG:HG2	1.89	0.72
1:A:931:GLN:HG2	1:A:950:ARG:NH1	2.05	0.71
1:C:389:LEU:HD13	1:C:421:LEU:HD23	1.73	0.71
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.17	0.71
1:A:335:VAL:HG13	1:A:414:THR:CG2	2.20	0.71
1:A:448:VAL:HA	1:A:456:ILE:HD13	1.73	0.71
1:B:451:ARG:HB3	1:B:456:ILE:HD11	1.73	0.71
1:A:750:GLU:HA	1:A:753:MET:HE3	1.73	0.70
1:B:750:GLU:HA	1:B:753:MET:HE3	1.73	0.70
1:D:372:VAL:HG22	1:D:432:ILE:CG2	2.21	0.70
1:C:1054:GLY:HA3	1:C:1153:ALA:H	1.56	0.70
1:A:94:MET:HG2	1:A:132:ILE:HD13	1.74	0.70
1:A:451:ARG:HB3	1:A:456:ILE:HD11	1.73	0.70
1:C:149:GLY:O	1:C:151:LEU:N	2.24	0.70
1:C:483:THR:HG21	1:C:498:LEU:HD21	1.73	0.70
1:A:389:LEU:HD13	1:A:421:LEU:HD23	1.72	0.70
1:C:750:GLU:HA	1:C:753:MET:HE3	1.73	0.70
1:A:483:THR:HG21	1:A:498:LEU:HD21	1.71	0.70
1:B:483:THR:HG21	1:B:498:LEU:HD21	1.72	0.70
1:B:227:ARG:HG3	1:B:288:GLU:CG	2.21	0.70
1:C:533:LYS:HA	1:C:603:MET:HE1	1.74	0.70
1:D:1025:MET:HE2	1:D:1025:MET:HA	1.74	0.70
1:C:574:TYR:CE1	1:D:439:GLU:HG2	2.26	0.70
1:D:548:VAL:O	1:D:549:LEU:HB3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:GLU:HA	1:D:753:MET:HE3	1.72	0.69
1:B:371:SER:OG	1:B:433:HIS:HE1	1.75	0.69
1:C:448:VAL:HA	1:C:456:ILE:HD13	1.74	0.69
1:C:548:VAL:O	1:C:549:LEU:HB3	1.89	0.69
1:D:448:VAL:HA	1:D:456:ILE:HD13	1.74	0.69
1:B:946:THR:HG22	1:B:950:ARG:HE	1.57	0.69
1:B:760:SER:HB2	1:B:766:LYS:HE2	1.75	0.69
1:C:946:THR:HG22	1:C:950:ARG:HE	1.57	0.69
1:C:1143:VAL:HG13	1:C:1206:LEU:HG	1.73	0.69
1:D:451:ARG:HB3	1:D:456:ILE:HD11	1.73	0.69
1:B:100:PHE:CD2	1:B:104:LEU:HB3	2.28	0.69
1:C:451:ARG:HB3	1:C:456:ILE:HD11	1.73	0.69
1:A:946:THR:HG22	1:A:950:ARG:HE	1.57	0.69
1:C:672:HIS:ND1	1:C:861:PRO:HG3	2.07	0.69
1:D:428:GLU:O	1:D:432:ILE:HG12	1.93	0.69
1:B:94:MET:HG2	1:B:129:LEU:HG	1.74	0.69
1:D:483:THR:HG21	1:D:498:LEU:HD21	1.74	0.68
1:D:760:SER:HB2	1:D:766:LYS:HE2	1.75	0.68
1:B:672:HIS:CE1	1:B:861:PRO:HG3	2.29	0.68
1:A:369:ARG:O	1:A:372:VAL:HG23	1.94	0.68
1:B:1025:MET:HA	1:B:1025:MET:HE2	1.74	0.68
1:B:1200:LYS:HB3	1:B:1274:LEU:HD21	1.74	0.68
1:C:1025:MET:HE2	1:C:1025:MET:HA	1.74	0.68
1:B:371:SER:OG	1:B:433:HIS:CE1	2.46	0.68
1:B:428:GLU:O	1:B:432:ILE:HG12	1.94	0.68
1:B:448:VAL:HA	1:B:456:ILE:HD13	1.75	0.68
1:B:369:ARG:O	1:B:372:VAL:HG23	1.94	0.68
1:D:946:THR:HG22	1:D:950:ARG:HE	1.57	0.68
1:D:1054:GLY:HA3	1:D:1153:ALA:H	1.58	0.67
1:A:760:SER:HB2	1:A:766:LYS:HE2	1.75	0.67
1:A:1055:ASP:N	1:A:1152:THR:HA	2.07	0.67
1:B:1143:VAL:HG13	1:B:1206:LEU:HG	1.75	0.67
1:A:1025:MET:HE2	1:A:1025:MET:HA	1.74	0.67
1:C:551:SER:C	1:D:277:PHE:HZ	2.02	0.67
1:A:838:MET:HE2	1:A:838:MET:HA	1.77	0.67
1:C:760:SER:HB2	1:C:766:LYS:HE2	1.75	0.67
1:A:65:ARG:HB3	1:A:100:PHE:CZ	2.30	0.67
1:A:1154:LEU:HD11	1:A:1163:LEU:HD12	1.76	0.67
1:B:1200:LYS:HB3	1:B:1274:LEU:CD2	2.25	0.67
1:D:759:ILE:HG22	1:D:760:SER:N	2.09	0.67
1:B:275:ILE:HD11	1:B:312:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1154:LEU:HD11	1:B:1163:LEU:HD12	1.76	0.67
1:D:275:ILE:HD11	1:D:312:LEU:HD11	1.75	0.67
1:B:713:ILE:HG21	1:B:772:SER:HB3	1.77	0.67
1:C:330:LEU:O	1:C:334:VAL:HG23	1.95	0.67
1:D:1154:LEU:HD11	1:D:1163:LEU:HD12	1.76	0.67
1:B:838:MET:HA	1:B:838:MET:HE2	1.76	0.67
1:A:908:LEU:HD22	1:A:980:LEU:HG	1.77	0.67
1:B:452:THR:HG22	1:D:452:THR:HG22	1.77	0.67
1:C:1190:GLY:N	1:C:1271:LYS:HZ1	1.93	0.67
1:A:470:ALA:HB3	1:A:473:ILE:HD11	1.77	0.67
1:A:759:ILE:HG22	1:A:760:SER:N	2.10	0.67
1:A:863:GLY:O	1:A:869:ILE:HD11	1.94	0.67
1:A:1190:GLY:N	1:A:1271:LYS:HZ1	1.93	0.67
1:D:330:LEU:O	1:D:334:VAL:HG23	1.95	0.67
1:A:347:SER:HB2	1:A:349:PHE:CE2	2.31	0.66
1:B:1259:TYR:CZ	1:B:1263:LEU:HD11	2.30	0.66
1:C:1195:VAL:O	1:C:1199:VAL:HG23	1.95	0.66
1:A:428:GLU:O	1:A:432:ILE:HG12	1.95	0.66
1:C:759:ILE:HG22	1:C:760:SER:N	2.09	0.66
1:D:369:ARG:O	1:D:372:VAL:HG23	1.95	0.66
1:D:838:MET:HE2	1:D:838:MET:HA	1.77	0.66
1:A:275:ILE:HD11	1:A:312:LEU:HD11	1.77	0.66
1:A:959:GLN:HB2	1:A:1005:TRP:CZ2	2.30	0.66
1:C:65:ARG:HB3	1:C:100:PHE:CZ	2.30	0.66
1:C:863:GLY:O	1:C:869:ILE:HD11	1.94	0.66
1:D:347:SER:HB2	1:D:349:PHE:CE2	2.31	0.66
1:B:1054:GLY:HA3	1:B:1153:ALA:H	1.58	0.66
1:C:470:ALA:HB3	1:C:473:ILE:HD11	1.77	0.66
1:C:959:GLN:HB2	1:C:1005:TRP:CZ2	2.30	0.66
1:C:1154:LEU:HD11	1:C:1163:LEU:HD12	1.76	0.66
1:A:1259:TYR:CZ	1:A:1263:LEU:HD11	2.30	0.66
1:B:863:GLY:O	1:B:869:ILE:HD11	1.95	0.66
1:D:1203:GLY:HA3	1:D:1278:MET:CG	2.26	0.66
1:A:475:GLN:HG3	1:A:476:ASN:H	1.61	0.66
1:B:297:GLN:CB	1:B:1104:GLY:HA3	2.26	0.66
1:B:712:MET:HE2	1:B:712:MET:HA	1.78	0.66
1:D:227:ARG:HG3	1:D:288:GLU:HG3	1.77	0.66
1:A:330:LEU:O	1:A:334:VAL:HG23	1.94	0.66
1:B:1203:GLY:HA3	1:B:1278:MET:HG2	1.78	0.66
1:D:1195:VAL:O	1:D:1199:VAL:HG23	1.96	0.66
1:A:169:TRP:CD1	1:A:169:TRP:H	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:VAL:O	1:A:1199:VAL:HG23	1.96	0.66
1:B:1195:VAL:O	1:B:1199:VAL:HG23	1.96	0.66
1:C:369:ARG:O	1:C:372:VAL:HG23	1.95	0.66
1:C:428:GLU:O	1:C:432:ILE:HG12	1.94	0.66
1:C:838:MET:HE2	1:C:838:MET:HA	1.77	0.66
1:D:959:GLN:HB2	1:D:1005:TRP:CZ2	2.31	0.66
1:C:33:LEU:HD23	1:C:75:LEU:HD11	1.78	0.65
1:C:275:ILE:HD11	1:C:312:LEU:HD11	1.77	0.65
1:D:863:GLY:O	1:D:869:ILE:HD11	1.95	0.65
1:B:475:GLN:HG3	1:B:476:ASN:H	1.62	0.65
1:B:759:ILE:HG22	1:B:760:SER:N	2.09	0.65
1:B:347:SER:HB2	1:B:349:PHE:CE2	2.30	0.65
1:C:347:SER:HB2	1:C:349:PHE:CE2	2.30	0.65
1:D:650:VAL:HG21	1:D:737:LYS:HG3	1.78	0.65
1:D:907:CYS:O	1:D:911:LEU:HB2	1.96	0.65
1:D:475:GLN:HG3	1:D:476:ASN:H	1.62	0.65
1:C:335:VAL:HG13	1:C:414:THR:HG21	1.79	0.65
1:D:1259:TYR:CZ	1:D:1263:LEU:HD11	2.31	0.65
1:B:169:TRP:CD1	1:B:169:TRP:H	2.14	0.65
1:B:290:LEU:O	1:B:294:LYS:HG3	1.97	0.65
1:C:1259:TYR:CZ	1:C:1263:LEU:HD11	2.32	0.65
1:A:226:ARG:HB2	1:A:288:GLU:HG2	1.77	0.65
1:A:377:HIS:H	1:A:377:HIS:HD2	1.45	0.65
1:C:169:TRP:CD1	1:C:169:TRP:H	2.15	0.65
1:C:475:GLN:HG3	1:C:476:ASN:H	1.61	0.65
1:C:1164:LEU:HB3	1:C:1252:LEU:HD21	1.79	0.65
1:D:169:TRP:CD1	1:D:169:TRP:H	2.15	0.65
1:B:330:LEU:O	1:B:334:VAL:HG23	1.96	0.64
1:C:907:CYS:O	1:C:911:LEU:HB2	1.97	0.64
1:A:907:CYS:O	1:A:911:LEU:HB2	1.96	0.64
1:B:470:ALA:HB3	1:B:473:ILE:HD11	1.78	0.64
1:D:120:ARG:HG2	1:D:172:ARG:NH1	2.13	0.64
1:D:470:ALA:HB3	1:D:473:ILE:HD11	1.80	0.64
1:B:959:GLN:HB2	1:B:1005:TRP:CZ2	2.32	0.64
1:C:121:LEU:C	1:C:123:ASN:H	2.06	0.64
1:C:298:GLN:HE21	1:C:336:LYS:HG2	1.63	0.64
1:D:712:MET:HE2	1:D:712:MET:HA	1.80	0.64
1:A:712:MET:HE2	1:A:712:MET:HA	1.78	0.64
1:B:548:VAL:HG11	1:B:580:GLU:O	1.97	0.64
1:C:712:MET:HE2	1:C:712:MET:HA	1.78	0.64
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:O	1:A:294:LYS:HG3	1.97	0.64
1:A:431:LYS:HE3	1:A:469:TYR:CE1	2.33	0.64
1:A:434:GLU:HG2	1:B:472:LEU:HD21	1.79	0.64
1:B:298:GLN:HE21	1:B:336:LYS:HG2	1.62	0.64
1:B:907:CYS:O	1:B:911:LEU:HB2	1.96	0.64
1:D:431:LYS:HE3	1:D:469:TYR:CE1	2.32	0.64
1:D:1160:VAL:O	1:D:1164:LEU:HG	1.98	0.64
1:B:121:LEU:C	1:B:123:ASN:H	2.05	0.64
1:B:377:HIS:H	1:B:377:HIS:HD2	1.46	0.64
1:D:548:VAL:HG11	1:D:580:GLU:O	1.96	0.64
1:B:671:GLN:OE1	1:B:672:HIS:CD2	2.50	0.63
1:D:1200:LYS:HB3	1:D:1274:LEU:HD21	1.79	0.63
1:D:1203:GLY:HA3	1:D:1278:MET:HG2	1.80	0.63
1:A:169:TRP:CD1	1:A:169:TRP:N	2.66	0.63
1:A:298:GLN:HE21	1:A:336:LYS:HG2	1.63	0.63
1:C:1160:VAL:O	1:C:1164:LEU:HG	1.98	0.63
1:D:245:ARG:NH1	1:D:366:GLU:OE2	2.31	0.63
1:B:169:TRP:H	1:B:169:TRP:HD1	1.47	0.63
1:B:372:VAL:HG22	1:B:432:ILE:CG2	2.28	0.63
1:B:1160:VAL:O	1:B:1164:LEU:HG	1.98	0.63
1:C:120:ARG:HG2	1:C:172:ARG:NH1	2.13	0.63
1:C:431:LYS:HE3	1:C:469:TYR:CE1	2.33	0.63
1:A:931:GLN:HG2	1:A:950:ARG:HH12	1.64	0.63
1:B:431:LYS:HE3	1:B:469:TYR:CE1	2.33	0.63
1:D:121:LEU:C	1:D:123:ASN:H	2.06	0.63
1:D:290:LEU:O	1:D:294:LYS:HG3	1.98	0.63
1:C:708:ILE:O	1:C:712:MET:HB2	1.99	0.63
1:A:1056:ILE:HD12	1:A:1216:TYR:CD1	2.34	0.62
1:B:413:MET:HA	1:B:413:MET:HE2	1.81	0.62
1:C:290:LEU:O	1:C:294:LYS:HG3	1.99	0.62
1:C:377:HIS:H	1:C:377:HIS:HD2	1.45	0.62
1:A:1198:LEU:HD22	1:A:1201:LEU:HD13	1.81	0.62
1:D:413:MET:HE2	1:D:413:MET:HA	1.81	0.62
1:B:120:ARG:HG2	1:B:172:ARG:NH1	2.13	0.62
1:B:169:TRP:CD1	1:B:169:TRP:N	2.66	0.62
1:D:169:TRP:CD1	1:D:169:TRP:N	2.67	0.62
1:A:121:LEU:C	1:A:123:ASN:H	2.05	0.62
1:C:499:LEU:HB3	1:C:541:LEU:HD13	1.82	0.62
1:B:245:ARG:NH1	1:B:366:GLU:OE2	2.32	0.62
1:C:413:MET:HE2	1:C:413:MET:HA	1.80	0.62
1:B:708:ILE:O	1:B:712:MET:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1046:SER:O	1:B:1050:HIS:HB3	1.99	0.62
1:C:1046:SER:O	1:C:1050:HIS:HB3	1.99	0.62
1:D:708:ILE:O	1:D:712:MET:HB2	1.99	0.62
1:A:94:MET:HG2	1:A:132:ILE:CD1	2.29	0.62
1:A:413:MET:HE2	1:A:413:MET:HA	1.81	0.62
1:B:609:TYR:CZ	1:B:613:ARG:HD2	2.35	0.62
1:B:1198:LEU:HD22	1:B:1201:LEU:HD13	1.81	0.62
1:C:377:HIS:CD2	1:C:377:HIS:N	2.67	0.62
1:D:372:VAL:HG22	1:D:432:ILE:HG21	1.82	0.62
1:D:1046:SER:O	1:D:1050:HIS:HB3	1.99	0.62
1:A:574:TYR:CE1	1:B:439:GLU:HG2	2.35	0.62
1:A:948:THR:HG23	1:A:992:LEU:HA	1.81	0.62
1:B:230:LEU:HD21	1:B:285:LEU:HD21	1.81	0.62
1:C:397:LYS:H	1:C:397:LYS:HD3	1.65	0.62
1:D:298:GLN:HE21	1:D:336:LYS:HG2	1.63	0.62
1:D:348:LYS:HG2	1:D:1035:TYR:O	2.00	0.62
1:A:190:GLU:O	1:A:194:VAL:HG23	2.00	0.62
1:A:377:HIS:CD2	1:A:377:HIS:N	2.67	0.62
1:B:65:ARG:HB3	1:B:100:PHE:CZ	2.31	0.62
1:B:650:VAL:HG21	1:B:737:LYS:HG3	1.82	0.62
1:D:245:ARG:HD2	1:D:366:GLU:OE1	2.00	0.62
1:D:609:TYR:CZ	1:D:613:ARG:HD2	2.34	0.62
1:A:708:ILE:O	1:A:712:MET:HB2	1.99	0.61
1:C:190:GLU:O	1:C:194:VAL:HG23	2.00	0.61
1:C:434:GLU:HG2	1:D:472:LEU:HD21	1.81	0.61
1:C:877:THR:OG1	1:C:914:THR:HG21	2.00	0.61
1:D:397:LYS:HD3	1:D:397:LYS:H	1.65	0.61
1:C:713:ILE:C	1:C:714:LYS:HG2	2.25	0.61
1:C:609:TYR:CZ	1:C:613:ARG:HD2	2.35	0.61
1:A:397:LYS:HD3	1:A:397:LYS:H	1.65	0.61
1:A:533:LYS:HA	1:A:603:MET:HE1	1.81	0.61
1:A:1179:LYS:HA	1:A:1182:LEU:HD12	1.82	0.61
1:B:948:THR:HG23	1:B:992:LEU:HA	1.81	0.61
1:D:190:GLU:O	1:D:194:VAL:HG23	2.00	0.61
1:D:948:THR:HG23	1:D:992:LEU:HA	1.82	0.61
1:D:1200:LYS:HB3	1:D:1274:LEU:CD2	2.31	0.61
1:B:713:ILE:C	1:B:714:LYS:HG2	2.25	0.61
1:B:877:THR:OG1	1:B:914:THR:HG21	2.00	0.61
1:C:169:TRP:CD1	1:C:169:TRP:N	2.67	0.61
1:C:472:LEU:HD21	1:D:434:GLU:HG2	1.82	0.61
1:C:713:ILE:HG21	1:C:772:SER:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:948:THR:HG23	1:C:992:LEU:HA	1.81	0.61
1:C:1198:LEU:HD22	1:C:1201:LEU:HD13	1.81	0.61
1:D:377:HIS:CD2	1:D:377:HIS:N	2.68	0.61
1:A:475:GLN:HG3	1:A:476:ASN:N	2.16	0.61
1:A:1160:VAL:O	1:A:1164:LEU:HG	1.99	0.61
1:B:190:GLU:O	1:B:194:VAL:HG23	2.00	0.61
1:B:377:HIS:CD2	1:B:377:HIS:N	2.68	0.61
1:C:33:LEU:HD22	1:C:75:LEU:HD21	1.81	0.61
1:A:348:LYS:HG2	1:A:1035:TYR:O	2.00	0.61
1:B:174:MET:HE1	1:B:205:LEU:HD11	1.82	0.61
1:D:169:TRP:H	1:D:169:TRP:HD1	1.47	0.61
1:A:609:TYR:CZ	1:A:613:ARG:HD2	2.35	0.61
1:B:779:LYS:O	1:B:783:ILE:HG13	2.01	0.61
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.82	0.61
1:D:338:PHE:CD2	1:D:414:THR:HG23	2.36	0.61
1:A:11:ASP:O	1:A:12:LYS:HG2	2.01	0.61
1:B:1179:LYS:HA	1:B:1182:LEU:HD12	1.82	0.61
1:D:187:THR:HG22	1:D:188:PRO:HD2	1.83	0.61
1:A:877:THR:OG1	1:A:914:THR:HG21	2.01	0.60
1:B:397:LYS:H	1:B:397:LYS:HD3	1.66	0.60
1:C:349:PHE:CD2	1:C:349:PHE:N	2.68	0.60
1:D:779:LYS:O	1:D:783:ILE:HG13	2.01	0.60
1:A:1046:SER:O	1:A:1050:HIS:HB3	1.99	0.60
1:C:13:THR:HA	1:C:17:LEU:HD12	1.83	0.60
1:B:499:LEU:HB3	1:B:541:LEU:HD13	1.82	0.60
1:B:1076:ALA:HA	1:B:1080:VAL:HB	1.83	0.60
1:C:1203:GLY:HA3	1:C:1278:MET:CG	2.30	0.60
1:D:713:ILE:C	1:D:714:LYS:HG2	2.25	0.60
1:D:1249:ILE:N	1:D:1250:PRO:HD2	2.16	0.60
1:B:100:PHE:O	1:B:105:LEU:HG	2.00	0.60
1:B:1249:ILE:N	1:B:1250:PRO:HD2	2.16	0.60
1:C:1076:ALA:HA	1:C:1080:VAL:HB	1.83	0.60
1:C:1249:ILE:N	1:C:1250:PRO:HD2	2.16	0.60
1:D:1198:LEU:HD22	1:D:1201:LEU:HD13	1.81	0.60
1:D:1076:ALA:HA	1:D:1080:VAL:HB	1.83	0.60
1:A:779:LYS:O	1:A:783:ILE:HG13	2.02	0.60
1:B:338:PHE:HD2	1:B:414:THR:HG23	1.65	0.60
1:A:499:LEU:HB3	1:A:541:LEU:HD13	1.83	0.60
1:A:713:ILE:C	1:A:714:LYS:HG2	2.26	0.60
1:B:475:GLN:HG3	1:B:476:ASN:N	2.16	0.60
1:C:11:ASP:O	1:C:12:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:MET:HE1	1:C:205:LEU:HD11	1.83	0.60
1:C:548:VAL:HG11	1:C:580:GLU:O	2.01	0.60
1:C:1179:LYS:HA	1:C:1182:LEU:HD12	1.82	0.60
1:D:529:LEU:HG	1:D:597:GLN:HG3	1.83	0.60
1:D:877:THR:OG1	1:D:914:THR:HG21	2.01	0.60
1:A:21:LEU:HD13	1:A:64:ARG:HD3	1.82	0.60
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.82	0.60
1:C:475:GLN:HG3	1:C:476:ASN:N	2.15	0.60
1:C:779:LYS:O	1:C:783:ILE:HG13	2.01	0.60
1:A:169:TRP:H	1:A:169:TRP:HD1	1.47	0.60
1:C:169:TRP:H	1:C:169:TRP:HD1	1.47	0.60
1:C:277:PHE:HZ	1:D:551:SER:C	2.10	0.60
1:C:480:VAL:O	1:C:483:THR:HB	2.02	0.60
1:D:174:MET:HE1	1:D:205:LEU:HD11	1.82	0.60
1:D:349:PHE:CD2	1:D:349:PHE:N	2.68	0.60
1:D:1179:LYS:HA	1:D:1182:LEU:HD12	1.82	0.60
1:B:1022:LYS:HA	1:B:1083:LEU:HD11	1.84	0.59
1:D:1022:LYS:HA	1:D:1083:LEU:HD11	1.84	0.59
1:D:1055:ASP:N	1:D:1152:THR:HA	2.17	0.59
1:A:72:CYS:HB2	1:A:93:LEU:HD11	1.84	0.59
1:A:124:GLY:O	1:A:127:LEU:N	2.36	0.59
1:A:930:LEU:HD13	1:A:950:ARG:HB2	1.84	0.59
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.16	0.59
1:A:174:MET:HE1	1:A:205:LEU:HD11	1.83	0.59
1:A:529:LEU:HG	1:A:597:GLN:HG3	1.84	0.59
1:B:187:THR:HG22	1:B:188:PRO:HD2	1.83	0.59
1:C:187:THR:HG22	1:C:188:PRO:HD2	1.83	0.59
1:C:989:SER:HB2	1:C:1031:LEU:HD21	1.83	0.59
1:C:1055:ASP:N	1:C:1152:THR:HA	2.13	0.59
1:D:480:VAL:O	1:D:483:THR:HB	2.03	0.59
1:A:13:THR:HA	1:A:17:LEU:HD12	1.84	0.59
1:B:361:SER:HG	1:B:417:HIS:CE1	2.20	0.59
1:C:570:VAL:HG21	1:D:376:ASP:HB2	1.83	0.59
1:D:230:LEU:HD21	1:D:285:LEU:HD21	1.83	0.59
1:D:741:CYS:O	1:D:745:ILE:HG13	2.03	0.59
1:A:480:VAL:O	1:A:483:THR:HB	2.03	0.59
1:D:499:LEU:HB3	1:D:541:LEU:HD13	1.82	0.59
1:A:672:HIS:HE1	1:A:805:SER:HB3	1.67	0.59
1:B:102:GLY:HA3	1:B:144:LEU:HD22	1.83	0.59
1:B:372:VAL:HG22	1:B:432:ILE:HG21	1.83	0.59
1:C:982:ILE:HD11	1:C:1024:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:HA3	1:C:144:LEU:HD22	1.85	0.59
1:A:18:GLN:HG2	1:A:53:GLY:O	2.03	0.59
1:A:518:LEU:HD11	1:D:518:LEU:HD11	1.85	0.58
1:B:671:GLN:OE1	1:B:672:HIS:HD2	1.85	0.58
1:C:551:SER:C	1:D:277:PHE:CZ	2.81	0.58
1:D:475:GLN:HG3	1:D:476:ASN:N	2.17	0.58
1:D:671:GLN:HE21	1:D:755:TYR:HA	1.68	0.58
1:D:1143:VAL:HG13	1:D:1206:LEU:HG	1.84	0.58
1:A:1087:GLN:O	1:A:1091:VAL:HG23	2.03	0.58
1:B:349:PHE:CD2	1:B:349:PHE:N	2.68	0.58
1:C:1022:LYS:HA	1:C:1083:LEU:HD11	1.85	0.58
1:D:102:GLY:HA3	1:D:144:LEU:HD22	1.85	0.58
1:D:227:ARG:HG3	1:D:288:GLU:CG	2.33	0.58
1:A:472:LEU:HD21	1:B:434:GLU:HG2	1.85	0.58
1:B:275:ILE:CD1	1:B:312:LEU:HD11	2.34	0.58
1:C:1200:LYS:HB3	1:C:1274:LEU:HD21	1.85	0.58
1:A:544:LYS:O	1:A:614:ARG:HD2	2.02	0.58
1:C:124:GLY:O	1:C:127:LEU:N	2.35	0.58
1:C:741:CYS:O	1:C:745:ILE:HG13	2.03	0.58
1:A:372:VAL:HG22	1:A:432:ILE:CG2	2.33	0.58
1:B:245:ARG:HD2	1:B:366:GLU:OE1	2.03	0.58
1:B:72:CYS:HB2	1:B:93:LEU:HD11	1.85	0.58
1:B:102:GLY:N	1:B:103:PRO:HD2	2.18	0.58
1:B:395:PRO:O	1:B:455:PRO:HG2	2.03	0.58
1:B:480:VAL:O	1:B:483:THR:HB	2.03	0.58
1:B:1164:LEU:HB3	1:B:1252:LEU:HD21	1.85	0.58
1:B:1055:ASP:N	1:B:1152:THR:HA	2.15	0.58
1:C:72:CYS:HB2	1:C:93:LEU:HD11	1.85	0.58
1:C:18:GLN:HG2	1:C:53:GLY:O	2.03	0.58
1:D:275:ILE:CD1	1:D:312:LEU:HD11	2.33	0.58
1:D:377:HIS:H	1:D:377:HIS:HD2	1.46	0.58
1:A:496:GLN:O	1:A:500:LYS:HG2	2.03	0.58
1:B:297:GLN:CG	1:B:1104:GLY:HA3	2.34	0.58
1:A:349:PHE:CD2	1:A:349:PHE:N	2.68	0.58
1:B:741:CYS:O	1:B:745:ILE:HG13	2.04	0.58
1:B:1087:GLN:O	1:B:1091:VAL:HG23	2.04	0.58
1:C:529:LEU:HG	1:C:597:GLN:HG3	1.85	0.58
1:A:102:GLY:HA3	1:A:144:LEU:HD22	1.85	0.57
1:A:1022:LYS:HA	1:A:1083:LEU:HD11	1.84	0.57
1:B:518:LEU:HD11	1:C:518:LEU:HD11	1.85	0.57
1:B:313:LEU:HB3	1:B:326:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ASP:O	1:C:304:CYS:N	2.38	0.57
1:D:496:GLN:O	1:D:500:LYS:HG2	2.04	0.57
1:D:835:GLY:HA2	1:D:838:MET:HB2	1.87	0.57
1:A:131:PRO:HA	1:A:184:VAL:HG22	1.87	0.57
1:A:1203:GLY:HA3	1:A:1278:MET:HG2	1.86	0.57
1:D:1087:GLN:O	1:D:1091:VAL:HG23	2.03	0.57
1:C:21:LEU:HD13	1:C:64:ARG:HD3	1.87	0.57
1:C:977:GLU:O	1:C:981:LEU:HB2	2.05	0.57
1:C:1203:GLY:HA3	1:C:1278:MET:HG2	1.86	0.57
1:A:102:GLY:N	1:A:103:PRO:HD2	2.20	0.57
1:A:671:GLN:CG	1:A:755:TYR:HB2	2.34	0.57
1:C:870:PHE:HD1	1:C:922:TYR:HD2	1.53	0.57
1:D:118:GLU:OE1	1:D:118:GLU:HA	2.05	0.57
1:D:300:ASP:O	1:D:304:CYS:N	2.38	0.57
1:A:741:CYS:O	1:A:745:ILE:HG13	2.05	0.57
1:C:496:GLN:O	1:C:500:LYS:HG2	2.05	0.57
1:C:650:VAL:HG21	1:C:737:LYS:HG3	1.85	0.57
1:D:131:PRO:HA	1:D:184:VAL:HG22	1.87	0.57
1:B:118:GLU:HA	1:B:118:GLU:OE1	2.05	0.56
1:B:131:PRO:HA	1:B:184:VAL:HG22	1.86	0.56
1:B:297:GLN:HG3	1:B:1104:GLY:HA3	1.87	0.56
1:B:977:GLU:O	1:B:981:LEU:HB2	2.04	0.56
1:C:430:PHE:CE2	1:C:466:ILE:HG23	2.40	0.56
1:C:1087:GLN:O	1:C:1091:VAL:HG23	2.05	0.56
1:D:259:ALA:HB3	1:D:260:PRO:CD	2.29	0.56
1:D:313:LEU:HB3	1:D:326:VAL:HG13	1.86	0.56
1:D:1190:GLY:N	1:D:1271:LYS:HZ1	2.03	0.56
1:A:300:ASP:O	1:A:304:CYS:N	2.38	0.56
1:A:439:GLU:HG2	1:B:574:TYR:CE1	2.39	0.56
1:A:593:SER:HB2	1:A:600:ILE:HG21	1.87	0.56
1:B:300:ASP:O	1:B:304:CYS:N	2.38	0.56
1:C:313:LEU:HB3	1:C:326:VAL:HG13	1.87	0.56
1:C:835:GLY:HA2	1:C:838:MET:HB2	1.87	0.56
1:D:102:GLY:N	1:D:103:PRO:HD2	2.20	0.56
1:D:977:GLU:O	1:D:981:LEU:HB2	2.05	0.56
1:A:430:PHE:CE2	1:A:466:ILE:HG23	2.40	0.56
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.05	0.56
1:B:496:GLN:O	1:B:500:LYS:HG2	2.05	0.56
1:C:1146:PHE:CE1	1:C:1170:ILE:HD11	2.41	0.56
1:D:1146:PHE:O	1:D:1150:VAL:HG23	2.06	0.56
1:B:870:PHE:HD1	1:B:922:TYR:HD2	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ILE:CD1	1:C:312:LEU:HD11	2.35	0.56
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.36	0.56
1:A:389:LEU:CD1	1:A:421:LEU:HD23	2.36	0.56
1:A:870:PHE:HD1	1:A:922:TYR:HD2	1.53	0.56
1:B:150:ASP:OD1	1:B:151:LEU:HG	2.06	0.56
1:B:593:SER:HB2	1:B:600:ILE:HG21	1.88	0.56
1:C:150:ASP:OD1	1:C:151:LEU:HG	2.06	0.56
1:D:870:PHE:HD1	1:D:922:TYR:HD2	1.53	0.56
1:B:103:PRO:HA	1:B:146:CYS:SG	2.45	0.56
1:C:102:GLY:N	1:C:103:PRO:HD2	2.21	0.56
1:C:194:VAL:O	1:C:198:VAL:HG23	2.06	0.56
1:C:1146:PHE:O	1:C:1150:VAL:HG23	2.06	0.56
1:D:103:PRO:HA	1:D:146:CYS:SG	2.46	0.56
1:A:313:LEU:HB3	1:A:326:VAL:HG13	1.87	0.56
1:B:124:GLY:O	1:B:127:LEU:N	2.37	0.56
1:D:799:VAL:O	1:D:847:GLN:CD	2.49	0.56
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.06	0.56
1:B:194:VAL:O	1:B:198:VAL:HG23	2.06	0.56
1:B:1146:PHE:O	1:B:1150:VAL:HG23	2.06	0.56
1:C:451:ARG:HB3	1:C:456:ILE:CD1	2.36	0.56
1:D:930:LEU:HD13	1:D:950:ARG:HB2	1.88	0.56
1:A:150:ASP:OD1	1:A:151:LEU:HG	2.06	0.55
1:A:194:VAL:O	1:A:198:VAL:HG23	2.06	0.55
1:B:908:LEU:HD11	1:B:981:LEU:HG	1.88	0.55
1:C:376:ASP:HB2	1:D:570:VAL:HG21	1.87	0.55
1:C:439:GLU:HG2	1:D:574:TYR:CE1	2.41	0.55
1:D:372:VAL:HG22	1:D:432:ILE:HG23	1.88	0.55
1:D:672:HIS:CE1	1:D:861:PRO:HG3	2.39	0.55
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.87	0.55
1:A:977:GLU:O	1:A:981:LEU:HB2	2.05	0.55
1:A:1146:PHE:CE1	1:A:1170:ILE:HD11	2.41	0.55
1:B:544:LYS:O	1:B:614:ARG:HD2	2.06	0.55
1:B:982:ILE:HD11	1:B:1024:LEU:HG	1.88	0.55
1:C:760:SER:HB2	1:C:766:LYS:CE	2.36	0.55
1:D:187:THR:CG2	1:D:188:PRO:HD2	2.37	0.55
1:D:451:ARG:HB3	1:D:456:ILE:CD1	2.35	0.55
1:D:1146:PHE:CE1	1:D:1170:ILE:HD11	2.41	0.55
1:A:65:ARG:HD3	1:A:100:PHE:CE1	2.41	0.55
1:A:384:GLU:O	1:A:388:ILE:HG13	2.07	0.55
1:A:395:PRO:O	1:A:455:PRO:HG2	2.05	0.55
1:A:661:GLU:OE1	1:A:666:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ASP:HB2	1:B:803:LEU:CD1	2.37	0.55
1:C:661:GLU:OE1	1:C:666:LEU:HD12	2.06	0.55
1:C:979:LEU:HD11	1:C:1019:SER:HB2	1.87	0.55
1:A:103:PRO:HA	1:A:146:CYS:SG	2.47	0.55
1:A:799:VAL:O	1:A:847:GLN:CD	2.50	0.55
1:B:1146:PHE:CE1	1:B:1170:ILE:HD11	2.41	0.55
1:C:65:ARG:HD3	1:C:100:PHE:CE1	2.42	0.55
1:C:131:PRO:HA	1:C:184:VAL:HG22	1.87	0.55
1:C:615:ASN:OD1	1:C:617:GLN:HG2	2.06	0.55
1:D:704:MET:O	1:D:708:ILE:HG13	2.07	0.55
1:D:760:SER:HB2	1:D:766:LYS:CE	2.36	0.55
1:A:479:LYS:HE2	1:A:482:GLU:OE1	2.07	0.55
1:A:760:SER:HB2	1:A:766:LYS:CE	2.36	0.55
1:B:187:THR:CG2	1:B:188:PRO:HD2	2.37	0.55
1:B:391:ASP:OD2	1:B:447:ARG:NH1	2.39	0.55
1:B:835:GLY:HA2	1:B:838:MET:HB2	1.87	0.55
1:D:124:GLY:O	1:D:127:LEU:N	2.38	0.55
1:B:451:ARG:HB3	1:B:456:ILE:CD1	2.35	0.55
1:D:479:LYS:HE2	1:D:482:GLU:OE1	2.07	0.55
1:D:593:SER:OG	1:D:604:LEU:HD22	2.07	0.55
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.88	0.55
1:B:479:LYS:HE2	1:B:482:GLU:OE1	2.06	0.55
1:B:593:SER:OG	1:B:604:LEU:HD22	2.07	0.55
1:C:103:PRO:HA	1:C:146:CYS:SG	2.46	0.55
1:D:194:VAL:O	1:D:198:VAL:HG23	2.06	0.55
1:D:826:GLU:O	1:D:830:VAL:HG23	2.07	0.55
1:D:826:GLU:HA	1:D:829:SER:HG	1.71	0.55
1:B:661:GLU:OE1	1:B:666:LEU:HD12	2.07	0.55
1:D:150:ASP:OD1	1:D:151:LEU:HG	2.06	0.55
1:D:1029:PHE:O	1:D:1033:VAL:HG23	2.07	0.55
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.36	0.55
1:A:372:VAL:HG22	1:A:432:ILE:HG21	1.88	0.55
1:A:483:THR:CG2	1:A:498:LEU:HD21	2.37	0.55
1:A:1054:GLY:CA	1:A:1152:THR:HG23	2.37	0.55
1:C:118:GLU:OE1	1:C:118:GLU:HA	2.07	0.55
1:D:176:GLN:O	1:D:180:VAL:HG23	2.07	0.55
1:D:430:PHE:CE2	1:D:466:ILE:HG23	2.42	0.55
1:A:451:ARG:HB3	1:A:456:ILE:CD1	2.36	0.54
1:B:176:GLN:O	1:B:180:VAL:HG23	2.07	0.54
1:B:826:GLU:O	1:B:830:VAL:HG23	2.07	0.54
1:C:187:THR:CG2	1:C:188:PRO:HD2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LYS:HE2	1:C:482:GLU:OE1	2.08	0.54
1:C:1185:CYS:SG	1:C:1191:ILE:HG12	2.47	0.54
1:D:337:SER:OG	1:D:359:CYS:HB2	2.07	0.54
1:A:176:GLN:O	1:A:180:VAL:HG23	2.08	0.54
1:A:671:GLN:OE1	1:A:672:HIS:HD2	1.91	0.54
1:B:430:PHE:CE2	1:B:466:ILE:HG23	2.42	0.54
1:C:150:ASP:O	1:C:151:LEU:HD23	2.07	0.54
1:D:353:LEU:HB3	1:D:1131:ILE:HG12	1.89	0.54
1:D:671:GLN:OE1	1:D:672:HIS:HD2	1.89	0.54
1:B:99:HIS:O	1:B:101:PRO:HD3	2.07	0.54
1:B:704:MET:O	1:B:708:ILE:HG13	2.07	0.54
1:B:760:SER:HB2	1:B:766:LYS:CE	2.36	0.54
1:A:1203:GLY:HA3	1:A:1278:MET:CG	2.37	0.54
1:D:661:GLU:OE1	1:D:666:LEU:HD12	2.08	0.54
1:D:713:ILE:HG21	1:D:772:SER:HB3	1.88	0.54
1:A:434:GLU:HA	1:A:437:ARG:HG3	1.90	0.54
1:A:593:SER:OG	1:A:604:LEU:HD22	2.08	0.54
1:B:337:SER:OG	1:B:359:CYS:HB2	2.08	0.54
1:C:574:TYR:OH	1:D:383:ILE:HD11	2.07	0.54
1:C:1029:PHE:O	1:C:1033:VAL:HG23	2.08	0.54
1:A:650:VAL:HG21	1:A:737:LYS:HG3	1.89	0.54
1:C:799:VAL:O	1:C:847:GLN:CD	2.49	0.54
1:C:826:GLU:O	1:C:830:VAL:HG23	2.08	0.54
1:D:446:ASN:O	1:D:450:THR:HB	2.08	0.54
1:D:548:VAL:O	1:D:569:ASP:HB3	2.08	0.54
1:A:966:LEU:O	1:A:1013:TYR:OH	2.26	0.54
1:B:766:LYS:HB2	1:B:766:LYS:NZ	2.23	0.54
1:C:383:ILE:HD11	1:D:574:TYR:OH	2.07	0.54
1:C:593:SER:HB2	1:C:600:ILE:HG21	1.88	0.54
1:C:704:MET:O	1:C:708:ILE:HG13	2.07	0.54
1:A:85:VAL:O	1:A:89:ILE:HG13	2.08	0.54
1:A:826:GLU:O	1:A:830:VAL:HG23	2.07	0.54
1:A:1029:PHE:O	1:A:1033:VAL:HG23	2.07	0.54
1:B:297:GLN:HB2	1:B:1104:GLY:HA3	1.90	0.54
1:B:499:LEU:HD13	1:B:538:GLY:HA2	1.90	0.54
1:B:513:ARG:O	1:B:517:ILE:HD12	2.08	0.54
1:B:1029:PHE:O	1:B:1033:VAL:HG23	2.07	0.54
1:C:176:GLN:O	1:C:180:VAL:HG23	2.07	0.54
1:D:499:LEU:HD13	1:D:538:GLY:HA2	1.90	0.54
1:B:384:GLU:O	1:B:388:ILE:HG13	2.09	0.53
1:B:615:ASN:OD1	1:B:617:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:ILE:CG2	1:B:772:SER:HB3	2.38	0.53
1:C:434:GLU:HA	1:C:437:ARG:HG3	1.89	0.53
1:A:760:SER:HB3	1:A:762:PHE:HD1	1.73	0.53
1:B:654:GLY:O	1:B:655:SER:OG	2.22	0.53
1:D:593:SER:HB2	1:D:600:ILE:HG21	1.89	0.53
1:D:667:LEU:HB3	1:D:751:VAL:HG11	1.90	0.53
1:A:1164:LEU:HB3	1:A:1252:LEU:HD21	1.90	0.53
1:D:533:LYS:HA	1:D:603:MET:HE1	1.89	0.53
1:D:544:LYS:O	1:D:614:ARG:HD2	2.08	0.53
1:D:524:MET:CB	1:D:592:ARG:HH21	2.22	0.53
1:C:337:SER:OG	1:C:359:CYS:HB2	2.08	0.53
1:C:389:LEU:CD1	1:C:421:LEU:HD23	2.38	0.53
1:D:815:ALA:O	1:D:819:ASP:HB3	2.09	0.53
1:A:671:GLN:OE1	1:A:672:HIS:CD2	2.62	0.53
1:A:815:ALA:O	1:A:819:ASP:HB3	2.09	0.53
1:B:529:LEU:HG	1:B:597:GLN:HG3	1.91	0.53
1:B:533:LYS:HA	1:B:603:MET:HE1	1.89	0.53
1:B:763:SER:O	1:B:767:PHE:HD1	1.92	0.53
1:D:391:ASP:OD2	1:D:447:ARG:NH1	2.42	0.53
1:D:671:GLN:OE1	1:D:672:HIS:CD2	2.62	0.53
1:D:766:LYS:HB2	1:D:766:LYS:NZ	2.23	0.53
1:D:908:LEU:HD22	1:D:980:LEU:HG	1.89	0.53
1:D:946:THR:HA	1:D:949:GLN:HB2	1.91	0.53
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.43	0.53
1:B:238:ARG:HE	1:B:306:CYS:HB3	1.74	0.53
1:B:368:VAL:HG11	1:B:428:GLU:HB3	1.91	0.53
1:B:446:ASN:O	1:B:450:THR:HB	2.07	0.53
1:C:384:GLU:O	1:C:388:ILE:HG13	2.08	0.53
1:C:593:SER:OG	1:C:604:LEU:HD22	2.08	0.53
1:C:826:GLU:HA	1:C:829:SER:HG	1.74	0.53
1:D:832:ARG:HA	1:D:838:MET:HG2	1.91	0.53
1:B:65:ARG:HD3	1:B:100:PHE:CE1	2.43	0.53
1:B:434:GLU:HA	1:B:437:ARG:HG3	1.90	0.53
1:B:467:ILE:HG12	1:B:474:LEU:HD12	1.90	0.53
1:B:483:THR:CG2	1:B:498:LEU:HD21	2.38	0.53
1:B:815:ALA:O	1:B:819:ASP:HB3	2.09	0.53
1:B:989:SER:HB2	1:B:1031:LEU:HD21	1.90	0.53
1:D:574:TYR:N	1:D:574:TYR:CD2	2.74	0.53
1:D:760:SER:HB3	1:D:762:PHE:HD1	1.74	0.53
1:A:615:ASN:OD1	1:A:617:GLN:HG2	2.08	0.53
1:B:210:ILE:N	1:B:211:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:ALA:O	1:C:819:ASP:HB3	2.09	0.53
1:D:434:GLU:HA	1:D:437:ARG:HG3	1.90	0.53
1:B:548:VAL:O	1:B:569:ASP:HB3	2.09	0.53
1:C:654:GLY:O	1:C:655:SER:OG	2.22	0.53
1:C:1055:ASP:O	1:C:1056:ILE:C	2.52	0.53
1:A:704:MET:O	1:A:708:ILE:HG13	2.08	0.52
1:C:766:LYS:HB2	1:C:766:LYS:NZ	2.23	0.52
1:A:446:ASN:O	1:A:450:THR:HB	2.09	0.52
1:A:467:ILE:HG12	1:A:474:LEU:HD12	1.90	0.52
1:B:755:TYR:CZ	1:B:759:ILE:HD11	2.45	0.52
1:B:946:THR:HA	1:B:949:GLN:HB2	1.91	0.52
1:C:446:ASN:O	1:C:450:THR:HB	2.07	0.52
1:C:467:ILE:HG12	1:C:474:LEU:HD12	1.90	0.52
1:C:946:THR:HA	1:C:949:GLN:HB2	1.91	0.52
1:D:513:ARG:O	1:D:517:ILE:HD12	2.09	0.52
1:D:908:LEU:HD11	1:D:981:LEU:HG	1.92	0.52
1:A:456:ILE:HG23	1:A:456:ILE:O	2.09	0.52
1:A:499:LEU:HD13	1:A:538:GLY:HA2	1.91	0.52
1:B:651:LEU:HD23	1:B:658:PHE:HB2	1.92	0.52
1:B:865:ASN:O	1:B:869:ILE:HG13	2.08	0.52
1:C:483:THR:CG2	1:C:498:LEU:HD21	2.38	0.52
1:C:499:LEU:HD13	1:C:538:GLY:HA2	1.91	0.52
1:C:1032:HIS:O	1:C:1035:TYR:N	2.37	0.52
1:D:923:GLN:HB3	1:D:924:PRO:HD3	1.92	0.52
1:A:828:LEU:HB3	1:A:832:ARG:HD3	1.91	0.52
1:B:100:PHE:CD2	1:B:104:LEU:HD13	2.45	0.52
1:C:763:SER:O	1:C:767:PHE:HD1	1.92	0.52
1:D:389:LEU:HD13	1:D:421:LEU:HD23	1.91	0.52
1:A:210:ILE:N	1:A:211:PRO:HD2	2.25	0.52
1:A:259:ALA:HB3	1:A:260:PRO:CD	2.29	0.52
1:C:1200:LYS:HB3	1:C:1274:LEU:CD2	2.39	0.52
1:D:865:ASN:O	1:D:869:ILE:HG13	2.09	0.52
1:D:1164:LEU:HB3	1:D:1252:LEU:HD21	1.90	0.52
1:A:766:LYS:HB2	1:A:766:LYS:NZ	2.23	0.52
1:A:1032:HIS:O	1:A:1035:TYR:N	2.36	0.52
1:B:832:ARG:HA	1:B:838:MET:HG2	1.92	0.52
1:B:1149:LEU:HB3	1:B:1163:LEU:HD11	1.92	0.52
1:C:85:VAL:O	1:C:89:ILE:HG13	2.09	0.52
1:D:210:ILE:N	1:D:211:PRO:HD2	2.24	0.52
1:A:54:SER:HB2	1:A:61:GLY:O	2.10	0.52
1:A:337:SER:OG	1:A:359:CYS:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:VAL:O	1:B:89:ILE:HG13	2.08	0.52
1:B:799:VAL:O	1:B:847:GLN:CD	2.50	0.52
1:B:1055:ASP:O	1:B:1056:ILE:C	2.52	0.52
1:C:54:SER:HB2	1:C:61:GLY:O	2.10	0.52
1:C:760:SER:HB3	1:C:762:PHE:HD1	1.73	0.52
1:C:923:GLN:HB3	1:C:924:PRO:HD3	1.92	0.52
1:D:1095:VAL:HG13	1:D:1135:ILE:HG23	1.90	0.52
1:A:865:ASN:O	1:A:869:ILE:HG13	2.10	0.52
1:A:1055:ASP:O	1:A:1056:ILE:C	2.52	0.52
1:B:121:LEU:C	1:B:123:ASN:N	2.68	0.52
1:C:383:ILE:HG22	1:C:429:THR:HG21	1.91	0.52
1:C:755:TYR:CZ	1:C:759:ILE:HD11	2.44	0.52
1:C:760:SER:HB2	1:C:766:LYS:HZ1	1.74	0.52
1:C:832:ARG:HA	1:C:838:MET:HG2	1.91	0.52
1:C:865:ASN:O	1:C:869:ILE:HG13	2.09	0.52
1:D:959:GLN:HB2	1:D:1005:TRP:CE2	2.45	0.52
1:A:763:SER:O	1:A:767:PHE:HD1	1.91	0.52
1:A:923:GLN:HB3	1:A:924:PRO:HD3	1.91	0.52
1:C:574:TYR:CZ	1:D:439:GLU:HG2	2.45	0.52
1:C:828:LEU:HB3	1:C:832:ARG:HD3	1.91	0.52
1:D:467:ILE:HG12	1:D:474:LEU:HD12	1.91	0.52
1:A:21:LEU:HB3	1:A:64:ARG:NE	2.25	0.52
1:B:574:TYR:CD2	1:B:574:TYR:N	2.75	0.52
1:B:760:SER:HB3	1:B:762:PHE:HD1	1.74	0.52
1:C:395:PRO:O	1:C:455:PRO:HG2	2.10	0.52
1:C:574:TYR:N	1:C:574:TYR:CD2	2.76	0.52
1:C:1149:LEU:HB3	1:C:1163:LEU:HD11	1.92	0.52
1:A:671:GLN:HG3	1:A:755:TYR:HB2	1.91	0.51
1:A:832:ARG:HA	1:A:838:MET:HG2	1.90	0.51
1:B:828:LEU:HB3	1:B:832:ARG:HD3	1.92	0.51
1:C:210:ILE:N	1:C:211:PRO:HD2	2.25	0.51
1:A:946:THR:HA	1:A:949:GLN:HB2	1.91	0.51
1:B:303:LYS:HG2	1:B:357:ARG:NH2	2.25	0.51
1:C:348:LYS:HG2	1:C:1035:TYR:O	2.10	0.51
1:C:510:MET:HG2	1:D:435:MET:HE2	1.91	0.51
1:C:651:LEU:HD23	1:C:658:PHE:HB2	1.91	0.51
1:C:959:GLN:HB2	1:C:1005:TRP:CE2	2.45	0.51
1:D:763:SER:O	1:D:767:PHE:HD1	1.92	0.51
1:D:1055:ASP:O	1:D:1056:ILE:C	2.53	0.51
1:A:672:HIS:CE1	1:A:805:SER:HB3	2.43	0.51
1:A:959:GLN:HB2	1:A:1005:TRP:CE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ILE:HG23	1:B:456:ILE:O	2.10	0.51
1:B:826:GLU:HA	1:B:829:SER:HG	1.74	0.51
1:B:908:LEU:HD22	1:B:980:LEU:HG	1.91	0.51
1:C:1056:ILE:HD12	1:C:1216:TYR:CG	2.45	0.51
1:D:303:LYS:HG2	1:D:357:ARG:NH2	2.26	0.51
1:D:651:LEU:HD23	1:D:658:PHE:HB2	1.92	0.51
1:A:1149:LEU:HB3	1:A:1163:LEU:HD11	1.92	0.51
1:C:1095:VAL:HG13	1:C:1135:ILE:HG23	1.93	0.51
1:A:551:SER:C	1:B:277:PHE:HZ	2.19	0.51
1:D:384:GLU:O	1:D:388:ILE:HG13	2.11	0.51
1:D:615:ASN:OD1	1:D:617:GLN:HG2	2.10	0.51
1:D:652:THR:OG1	1:D:657:ILE:HG12	2.11	0.51
1:A:60:ASP:O	1:A:64:ARG:HB2	2.11	0.51
1:C:652:THR:OG1	1:C:657:ILE:HG12	2.11	0.51
1:C:966:LEU:HB3	1:C:1013:TYR:CZ	2.46	0.51
1:B:361:SER:OG	1:B:417:HIS:CE1	2.64	0.51
1:D:931:GLN:HG2	1:D:950:ARG:NH1	2.26	0.51
1:A:303:LYS:HG2	1:A:357:ARG:NH2	2.26	0.51
1:B:297:GLN:CG	1:B:1104:GLY:CA	2.88	0.51
1:B:639:ASP:H	1:B:711:ARG:HE	1.59	0.51
1:B:959:GLN:HB2	1:B:1005:TRP:CE2	2.46	0.51
1:C:456:ILE:O	1:C:456:ILE:HG23	2.09	0.51
1:D:297:GLN:HG3	1:D:1104:GLY:HA2	1.93	0.51
1:A:72:CYS:CB	1:A:93:LEU:HD11	2.40	0.51
1:B:66:TYR:CE1	1:B:107:ASP:HB3	2.47	0.51
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.29	0.51
1:C:1054:GLY:CA	1:C:1152:THR:HG23	2.41	0.51
1:A:394:GLY:O	1:A:396:LYS:HE3	2.11	0.50
1:A:513:ARG:O	1:A:517:ILE:HD12	2.11	0.50
1:B:979:LEU:HD11	1:B:1019:SER:HB2	1.93	0.50
1:C:146:CYS:O	1:C:147:GLY:C	2.54	0.50
1:C:743:CYS:HA	1:C:746:MET:HB2	1.94	0.50
1:D:121:LEU:C	1:D:123:ASN:N	2.69	0.50
1:D:755:TYR:CZ	1:D:759:ILE:HD11	2.46	0.50
1:D:1273:ASN:O	1:D:1276:GLN:N	2.44	0.50
1:A:33:LEU:HD22	1:A:75:LEU:HD21	1.92	0.50
1:A:839:HIS:HB3	1:A:903:ILE:HG13	1.93	0.50
1:D:1056:ILE:HD12	1:D:1216:TYR:CG	2.47	0.50
1:A:651:LEU:HD23	1:A:658:PHE:HB2	1.92	0.50
1:A:743:CYS:HA	1:A:746:MET:HB2	1.93	0.50
1:A:995:THR:O	1:A:996:SER:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:SER:O	1:A:1090:LYS:HG2	2.12	0.50
1:B:72:CYS:CB	1:B:93:LEU:HD11	2.41	0.50
1:C:348:LYS:HD3	1:C:1034:LEU:O	2.10	0.50
1:D:1149:LEU:HB3	1:D:1163:LEU:HD11	1.92	0.50
1:A:1050:HIS:HA	1:A:1152:THR:OG1	2.12	0.50
1:B:382:LEU:HD22	1:B:425:ILE:HG23	1.92	0.50
1:B:652:THR:OG1	1:B:657:ILE:HG12	2.11	0.50
1:B:743:CYS:HA	1:B:746:MET:HB2	1.93	0.50
1:C:216:GLN:O	1:C:219:VAL:HG22	2.12	0.50
1:D:483:THR:CG2	1:D:498:LEU:HD21	2.40	0.50
1:D:839:HIS:HB3	1:D:903:ILE:HG13	1.94	0.50
1:A:652:THR:OG1	1:A:657:ILE:HG12	2.11	0.50
1:B:839:HIS:HB3	1:B:903:ILE:HG13	1.94	0.50
1:B:923:GLN:HB3	1:B:924:PRO:HD3	1.92	0.50
1:C:72:CYS:CB	1:C:93:LEU:HD11	2.41	0.50
1:C:839:HIS:HB3	1:C:903:ILE:HG13	1.93	0.50
1:D:395:PRO:O	1:D:455:PRO:HG2	2.12	0.50
1:D:456:ILE:HG23	1:D:456:ILE:O	2.10	0.50
1:A:1054:GLY:HA3	1:A:1152:THR:HG23	1.93	0.50
1:A:1056:ILE:HD12	1:A:1216:TYR:CG	2.47	0.50
1:B:262:ASP:O	1:B:266:HIS:ND1	2.44	0.50
1:B:993:GLU:CD	1:B:994:PRO:HD2	2.37	0.50
1:C:303:LYS:HG2	1:C:357:ARG:NH2	2.26	0.50
1:C:513:ARG:O	1:C:517:ILE:HD12	2.12	0.50
1:C:713:ILE:O	1:C:714:LYS:CG	2.52	0.50
1:D:995:THR:O	1:D:996:SER:O	2.30	0.50
1:A:397:LYS:HD3	1:A:397:LYS:N	2.27	0.50
1:A:511:SER:O	1:A:515:SER:HB2	2.12	0.50
1:A:993:GLU:CD	1:A:994:PRO:HD2	2.37	0.50
1:B:94:MET:CG	1:B:129:LEU:HG	2.41	0.50
1:B:657:ILE:HD12	1:B:733:ASN:O	2.12	0.50
1:B:760:SER:HB2	1:B:766:LYS:HZ1	1.76	0.50
1:B:995:THR:O	1:B:996:SER:O	2.30	0.50
1:B:1032:HIS:O	1:B:1035:TYR:N	2.37	0.50
1:B:1054:GLY:O	1:B:1055:ASP:CB	2.59	0.50
1:C:275:ILE:O	1:C:279:ILE:HG13	2.11	0.50
1:D:828:LEU:HB3	1:D:832:ARG:HD3	1.91	0.50
1:D:843:ASN:O	1:D:847:GLN:HB2	2.12	0.50
1:A:732:THR:O	1:A:736:ILE:HG13	2.12	0.50
1:A:1252:LEU:O	1:A:1256:ILE:HG13	2.12	0.50
1:B:394:GLY:O	1:B:396:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1054:GLY:CA	1:B:1152:THR:HG23	2.41	0.50
1:D:639:ASP:H	1:D:711:ARG:HE	1.60	0.50
1:D:973:PHE:CD1	1:D:974:ASN:N	2.72	0.50
1:A:187:THR:HG22	1:A:188:PRO:CD	2.41	0.50
1:A:322:PHE:O	1:A:326:VAL:HG23	2.12	0.50
1:A:393:TYR:HB3	1:A:415:ASN:O	2.11	0.50
1:B:1092:LEU:HD13	1:B:1169:LYS:HG2	1.94	0.50
1:C:1252:LEU:O	1:C:1256:ILE:HG13	2.12	0.50
1:D:705:LEU:HB3	1:D:755:TYR:CE2	2.47	0.50
1:D:1086:SER:O	1:D:1090:LYS:HG2	2.12	0.50
1:B:227:ARG:HH21	1:B:291:LYS:HD3	1.77	0.49
1:C:639:ASP:H	1:C:711:ARG:HE	1.60	0.49
1:C:1092:LEU:HD13	1:C:1169:LYS:HG2	1.93	0.49
1:A:435:MET:HE2	1:B:510:MET:HG2	1.93	0.49
1:A:448:VAL:HA	1:A:456:ILE:CD1	2.42	0.49
1:A:654:GLY:O	1:A:655:SER:OG	2.22	0.49
1:B:227:ARG:CG	1:B:288:GLU:HG3	2.39	0.49
1:B:1086:SER:O	1:B:1090:LYS:HG2	2.12	0.49
1:C:993:GLU:CD	1:C:994:PRO:HD2	2.37	0.49
1:D:146:CYS:O	1:D:147:GLY:C	2.55	0.49
1:D:511:SER:O	1:D:515:SER:HB2	2.12	0.49
1:D:993:GLU:CD	1:D:994:PRO:HD2	2.37	0.49
1:A:216:GLN:O	1:A:219:VAL:HG22	2.11	0.49
1:A:589:SER:O	1:A:592:ARG:HG2	2.12	0.49
1:A:1002:MET:HG3	1:A:1031:LEU:CD1	2.42	0.49
1:B:146:CYS:O	1:B:147:GLY:C	2.55	0.49
1:C:187:THR:HG22	1:C:188:PRO:CD	2.41	0.49
1:D:838:MET:HA	1:D:838:MET:CE	2.42	0.49
1:A:552:LEU:HD23	1:A:552:LEU:C	2.38	0.49
1:B:1252:LEU:O	1:B:1256:ILE:HG13	2.12	0.49
1:C:1086:SER:O	1:C:1090:LYS:HG2	2.12	0.49
1:D:341:LEU:CD1	1:D:359:CYS:HB3	2.42	0.49
1:A:298:GLN:C	1:A:301:PRO:HD2	2.38	0.49
1:A:843:ASN:O	1:A:847:GLN:HB2	2.12	0.49
1:A:1054:GLY:HA3	1:A:1153:ALA:N	2.24	0.49
1:B:275:ILE:O	1:B:279:ILE:HG13	2.12	0.49
1:C:268:GLU:O	1:C:272:ILE:HG13	2.12	0.49
1:C:298:GLN:C	1:C:301:PRO:HD2	2.38	0.49
1:A:14:THR:O	1:A:15:ASP:C	2.55	0.49
1:A:275:ILE:O	1:A:279:ILE:HG13	2.12	0.49
1:A:435:MET:HG3	1:B:508:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:MET:CB	1:B:592:ARG:HH21	2.26	0.49
1:B:843:ASN:O	1:B:847:GLN:HB2	2.12	0.49
1:C:94:MET:HG2	1:C:132:ILE:HD13	1.94	0.49
1:C:397:LYS:HD3	1:C:397:LYS:N	2.27	0.49
1:C:995:THR:O	1:C:996:SER:O	2.30	0.49
1:C:1050:HIS:HA	1:C:1152:THR:OG1	2.12	0.49
1:D:201:MET:O	1:D:205:LEU:HD12	2.13	0.49
1:D:743:CYS:HA	1:D:746:MET:HB2	1.93	0.49
1:A:146:CYS:O	1:A:147:GLY:C	2.55	0.49
1:A:915:PHE:CE2	1:A:988:LEU:HD21	2.48	0.49
1:B:201:MET:O	1:B:205:LEU:HD12	2.13	0.49
1:B:1053:LEU:HD21	1:B:1077:ALA:HB2	1.95	0.49
1:C:230:LEU:HD21	1:C:285:LEU:HD21	1.94	0.49
1:C:322:PHE:O	1:C:326:VAL:HG23	2.13	0.49
1:C:930:LEU:HD13	1:C:950:ARG:HB2	1.94	0.49
1:C:1273:ASN:O	1:C:1276:GLN:N	2.45	0.49
1:D:238:ARG:HE	1:D:306:CYS:HB3	1.78	0.49
1:D:826:GLU:HA	1:D:829:SER:OG	2.13	0.49
1:D:976:LYS:O	1:D:980:LEU:HD22	2.13	0.49
1:D:1053:LEU:HD21	1:D:1077:ALA:HB2	1.95	0.49
1:A:1:MET:O	1:A:5:ILE:HG13	2.13	0.49
1:A:33:LEU:HD23	1:A:75:LEU:HD11	1.94	0.49
1:A:524:MET:CB	1:A:592:ARG:HH21	2.26	0.49
1:A:760:SER:HB2	1:A:766:LYS:NZ	2.28	0.49
1:B:77:GLU:OE1	1:B:121:LEU:CD2	2.57	0.49
1:B:760:SER:HB2	1:B:766:LYS:NZ	2.28	0.49
1:C:137:LEU:O	1:C:153:GLY:HA3	2.13	0.49
1:C:259:ALA:HB3	1:C:260:PRO:CD	2.29	0.49
1:C:394:GLY:O	1:C:396:LYS:HE3	2.12	0.49
1:C:760:SER:HB2	1:C:766:LYS:NZ	2.28	0.49
1:C:1054:GLY:O	1:C:1055:ASP:CB	2.59	0.49
1:D:1252:LEU:O	1:D:1256:ILE:HG13	2.12	0.49
1:A:826:GLU:HA	1:A:829:SER:OG	2.13	0.49
1:A:1092:LEU:HD13	1:A:1169:LYS:HG2	1.95	0.49
1:B:66:TYR:HE1	1:B:107:ASP:HB3	1.78	0.49
1:B:732:THR:O	1:B:736:ILE:HG13	2.13	0.49
1:B:1273:ASN:O	1:B:1276:GLN:N	2.44	0.49
1:C:826:GLU:HA	1:C:829:SER:OG	2.13	0.49
1:D:216:GLN:O	1:D:219:VAL:HG22	2.13	0.49
1:D:397:LYS:HD3	1:D:397:LYS:N	2.27	0.49
1:A:639:ASP:H	1:A:711:ARG:HE	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.93	0.49
1:A:1156:SER:HB3	1:A:1220:LYS:HE3	1.95	0.49
1:B:187:THR:HG22	1:B:188:PRO:CD	2.42	0.49
1:B:511:SER:O	1:B:515:SER:HB2	2.12	0.49
1:B:623:MET:HE1	1:B:673:CYS:CB	2.40	0.49
1:B:1054:GLY:HA3	1:B:1152:THR:HG23	1.95	0.49
1:C:21:LEU:HB3	1:C:64:ARG:NE	2.28	0.49
1:C:341:LEU:CD1	1:C:359:CYS:HB3	2.42	0.49
1:A:760:SER:HB2	1:A:766:LYS:HZ1	1.77	0.48
1:B:397:LYS:HD3	1:B:397:LYS:N	2.27	0.48
1:B:713:ILE:O	1:B:714:LYS:CG	2.53	0.48
1:C:201:MET:O	1:C:205:LEU:HD12	2.13	0.48
1:C:775:THR:O	1:C:779:LYS:HB2	2.13	0.48
1:D:275:ILE:O	1:D:279:ILE:HG13	2.13	0.48
1:D:635:GLU:O	1:D:711:ARG:NH2	2.40	0.48
1:D:1032:HIS:O	1:D:1035:TYR:N	2.37	0.48
1:D:1054:GLY:O	1:D:1055:ASP:CB	2.59	0.48
1:A:1273:ASN:O	1:A:1276:GLN:N	2.45	0.48
1:C:74:GLN:HA	1:C:77:GLU:OE2	2.13	0.48
1:D:552:LEU:C	1:D:552:LEU:HD23	2.37	0.48
1:D:760:SER:HB2	1:D:766:LYS:NZ	2.29	0.48
1:A:74:GLN:HA	1:A:77:GLU:OE2	2.14	0.48
1:A:548:VAL:HG11	1:A:580:GLU:O	2.14	0.48
1:A:635:GLU:O	1:A:711:ARG:NH2	2.39	0.48
1:A:1200:LYS:HB3	1:A:1274:LEU:HD21	1.96	0.48
1:A:1207:THR:O	1:A:1211:TYR:HD1	1.97	0.48
1:C:1:MET:O	1:C:5:ILE:HG13	2.13	0.48
1:C:870:PHE:CD1	1:C:922:TYR:HD2	2.32	0.48
1:D:187:THR:HG22	1:D:188:PRO:CD	2.42	0.48
1:D:298:GLN:C	1:D:301:PRO:HD2	2.38	0.48
1:A:201:MET:O	1:A:205:LEU:HD12	2.13	0.48
1:A:262:ASP:O	1:A:266:HIS:ND1	2.43	0.48
1:A:383:ILE:HD11	1:B:574:TYR:OH	2.13	0.48
1:A:574:TYR:CZ	1:B:439:GLU:HG2	2.48	0.48
1:B:74:GLN:HA	1:B:77:GLU:OE2	2.14	0.48
1:B:225:SER:O	1:B:226:ARG:C	2.57	0.48
1:C:816:LEU:CD1	1:C:838:MET:HE1	2.39	0.48
1:D:316:LEU:O	1:D:316:LEU:HD22	2.13	0.48
1:D:549:LEU:HD23	1:D:569:ASP:OD1	2.13	0.48
1:D:775:THR:O	1:D:779:LYS:HB2	2.14	0.48
1:D:816:LEU:CD1	1:D:838:MET:HE1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:NH1	1:A:878:ARG:HD2	2.29	0.48
1:A:1091:VAL:HA	1:A:1094:GLU:HG3	1.95	0.48
1:B:216:GLN:O	1:B:219:VAL:HG22	2.13	0.48
1:C:511:SER:O	1:C:515:SER:HB2	2.13	0.48
1:C:976:LYS:O	1:C:980:LEU:HD22	2.13	0.48
1:C:1207:THR:O	1:C:1211:TYR:HD1	1.97	0.48
1:D:394:GLY:O	1:D:396:LYS:HE3	2.12	0.48
1:D:713:ILE:O	1:D:714:LYS:CG	2.52	0.48
1:D:1054:GLY:CA	1:D:1152:THR:HG23	2.44	0.48
1:D:1091:VAL:HA	1:D:1094:GLU:HG3	1.95	0.48
1:A:341:LEU:CD1	1:A:359:CYS:HB3	2.43	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
1:B:298:GLN:C	1:B:301:PRO:HD2	2.38	0.48
1:B:503:GLN:HB2	1:B:504:PRO:HD3	1.96	0.48
1:B:552:LEU:HD23	1:B:552:LEU:C	2.38	0.48
1:B:816:LEU:CD1	1:B:838:MET:HE1	2.37	0.48
1:B:828:LEU:O	1:B:832:ARG:HG3	2.14	0.48
1:C:141:LYS:O	1:C:142:GLU:HG3	2.13	0.48
1:C:552:LEU:HD23	1:C:552:LEU:C	2.38	0.48
1:C:732:THR:O	1:C:736:ILE:HG13	2.14	0.48
1:C:1053:LEU:HD21	1:C:1077:ALA:HB2	1.95	0.48
1:D:732:THR:O	1:D:736:ILE:HG13	2.13	0.48
1:A:268:GLU:O	1:A:272:ILE:HG13	2.13	0.48
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.95	0.48
1:B:359:CYS:SG	1:B:361:SER:HB2	2.54	0.48
1:B:776:CYS:O	1:B:780:PHE:HD1	1.97	0.48
1:D:776:CYS:O	1:D:780:PHE:HD1	1.97	0.48
1:D:828:LEU:O	1:D:832:ARG:HG3	2.13	0.48
1:D:931:GLN:HG2	1:D:950:ARG:HH12	1.79	0.48
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.96	0.48
1:A:359:CYS:SG	1:A:361:SER:HB2	2.54	0.48
1:A:801:ASP:N	1:A:801:ASP:OD1	2.47	0.48
1:B:170:PRO:HG2	1:B:173:TYR:HD1	1.79	0.48
1:B:1080:VAL:O	1:B:1080:VAL:HG12	2.14	0.48
1:C:435:MET:HE2	1:D:510:MET:HG2	1.96	0.48
1:C:828:LEU:O	1:C:832:ARG:HG3	2.13	0.48
1:C:908:LEU:HD22	1:C:980:LEU:HG	1.96	0.48
1:D:225:SER:O	1:D:226:ARG:C	2.56	0.48
1:D:338:PHE:HD2	1:D:414:THR:HG23	1.77	0.48
1:D:589:SER:O	1:D:592:ARG:HG2	2.13	0.48
1:D:818:ARG:NH1	1:D:878:ARG:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:THR:O	1:A:779:LYS:HB2	2.14	0.48
1:A:985:LEU:HB3	1:A:1002:MET:HE1	1.95	0.48
1:B:137:LEU:O	1:B:153:GLY:HA3	2.14	0.48
1:B:448:VAL:HA	1:B:456:ILE:CD1	2.42	0.48
1:C:8:LEU:HD13	1:C:17:LEU:HA	1.96	0.48
1:C:540:LEU:HD13	1:C:607:GLY:HA3	1.95	0.48
1:A:671:GLN:HG2	1:A:755:TYR:HB2	1.96	0.48
1:B:341:LEU:CD1	1:B:359:CYS:HB3	2.43	0.48
1:B:826:GLU:HA	1:B:829:SER:OG	2.13	0.48
1:C:14:THR:O	1:C:15:ASP:C	2.56	0.48
1:C:170:PRO:HG2	1:C:173:TYR:HD1	1.79	0.48
1:C:806:LEU:CD2	1:C:872:ASN:HB3	2.44	0.48
1:D:137:LEU:O	1:D:153:GLY:HA3	2.13	0.48
1:D:672:HIS:HE1	1:D:805:SER:HB3	1.79	0.48
1:A:806:LEU:CD2	1:A:872:ASN:HB3	2.44	0.47
1:A:966:LEU:HB3	1:A:1013:TYR:CZ	2.49	0.47
1:A:1077:ALA:CB	1:A:1078:PRO:HD3	2.40	0.47
1:B:818:ARG:NH1	1:B:878:ARG:HD2	2.28	0.47
1:B:1091:VAL:HA	1:B:1094:GLU:HG3	1.95	0.47
1:B:1207:THR:O	1:B:1211:TYR:HD1	1.97	0.47
1:C:843:ASN:O	1:C:847:GLN:HB2	2.13	0.47
1:C:1054:GLY:HA3	1:C:1152:THR:HG23	1.95	0.47
1:D:268:GLU:O	1:D:272:ILE:HG13	2.14	0.47
1:A:503:GLN:HB2	1:A:504:PRO:HD3	1.96	0.47
1:A:828:LEU:O	1:A:832:ARG:HG3	2.13	0.47
1:B:268:GLU:O	1:B:272:ILE:HG13	2.14	0.47
1:B:806:LEU:CD2	1:B:872:ASN:HB3	2.44	0.47
1:B:976:LYS:O	1:B:980:LEU:HD22	2.13	0.47
1:B:985:LEU:HB3	1:B:1002:MET:HE1	1.96	0.47
1:D:170:PRO:HG2	1:D:173:TYR:HD1	1.79	0.47
1:D:259:ALA:CB	1:D:260:PRO:CD	2.91	0.47
1:D:594:LEU:HG	1:D:604:LEU:HD23	1.96	0.47
1:D:1050:HIS:HA	1:D:1152:THR:OG1	2.14	0.47
1:A:137:LEU:O	1:A:153:GLY:HA3	2.13	0.47
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.49	0.47
1:A:623:MET:HE1	1:A:673:CYS:CB	2.39	0.47
1:B:372:VAL:HG22	1:B:432:ILE:HG23	1.96	0.47
1:B:635:GLU:O	1:B:711:ARG:NH2	2.39	0.47
1:B:775:THR:O	1:B:779:LYS:HB2	2.14	0.47
1:C:604:LEU:HG	1:C:608:PHE:CE1	2.50	0.47
1:C:776:CYS:O	1:C:780:PHE:HD1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:918:VAL:HG21	1:C:929:PHE:CE2	2.50	0.47
1:D:359:CYS:SG	1:D:361:SER:HB2	2.54	0.47
1:A:705:LEU:HB3	1:A:755:TYR:CE2	2.49	0.47
1:B:589:SER:O	1:B:592:ARG:HG2	2.13	0.47
1:C:435:MET:HG3	1:D:508:ILE:O	2.14	0.47
1:C:1091:VAL:HA	1:C:1094:GLU:HG3	1.95	0.47
1:D:322:PHE:O	1:D:326:VAL:HG23	2.15	0.47
1:D:985:LEU:HB3	1:D:1002:MET:HE1	1.95	0.47
1:D:1207:THR:O	1:D:1211:TYR:HD1	1.97	0.47
1:A:174:MET:HA	1:A:177:LEU:HB2	1.96	0.47
1:B:581:THR:HB	1:B:585:GLU:HG3	1.97	0.47
1:B:870:PHE:CD1	1:B:922:TYR:HD2	2.32	0.47
1:C:581:THR:HB	1:C:585:GLU:HG3	1.96	0.47
1:D:1054:GLY:HA3	1:D:1152:THR:HG23	1.96	0.47
1:D:1080:VAL:O	1:D:1080:VAL:HG12	2.14	0.47
1:C:589:SER:O	1:C:592:ARG:HG2	2.13	0.47
1:D:271:VAL:O	1:D:275:ILE:HG23	2.15	0.47
1:A:439:GLU:HG2	1:B:574:TYR:CZ	2.49	0.47
1:A:776:CYS:O	1:A:780:PHE:HD1	1.97	0.47
1:A:1145:PHE:HD2	1:A:1146:PHE:CD1	2.33	0.47
1:B:226:ARG:NH1	1:B:282:ASP:CG	2.73	0.47
1:B:672:HIS:CE1	1:B:861:PRO:CG	2.96	0.47
1:B:966:LEU:HB3	1:B:1013:TYR:CZ	2.50	0.47
1:B:1095:VAL:HG13	1:B:1135:ILE:HG23	1.97	0.47
1:C:360:VAL:O	1:C:364:ILE:HG13	2.15	0.47
1:C:1145:PHE:HD2	1:C:1146:PHE:CD1	2.33	0.47
1:D:503:GLN:HB2	1:D:504:PRO:HD3	1.97	0.47
1:D:654:GLY:O	1:D:655:SER:OG	2.22	0.47
1:D:1145:PHE:HD2	1:D:1146:PHE:CD1	2.33	0.47
1:A:1150:VAL:HG12	1:A:1209:VAL:HG12	1.96	0.47
1:C:503:GLN:HB2	1:C:504:PRO:HD3	1.97	0.47
1:C:922:TYR:N	1:C:922:TYR:CD1	2.83	0.47
1:D:598:ALA:HA	1:D:601:ARG:HD3	1.96	0.47
1:A:918:VAL:HG21	1:A:929:PHE:CE2	2.50	0.47
1:A:1080:VAL:O	1:A:1080:VAL:HG12	2.14	0.47
1:B:922:TYR:N	1:B:922:TYR:CD1	2.83	0.47
1:C:121:LEU:C	1:C:123:ASN:N	2.69	0.47
1:C:818:ARG:NH1	1:C:878:ARG:HD2	2.29	0.47
1:C:908:LEU:HD11	1:C:981:LEU:HG	1.96	0.47
1:D:262:ASP:O	1:D:266:HIS:ND1	2.43	0.47
1:D:448:VAL:HA	1:D:456:ILE:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:806:LEU:CD2	1:D:872:ASN:HB3	2.44	0.47
1:D:911:LEU:CD2	1:D:915:PHE:HE1	2.28	0.47
1:A:339:LYS:HA	1:A:339:LYS:HD2	1.67	0.47
1:A:393:TYR:CD1	1:A:418:ALA:HB1	2.49	0.47
1:A:549:LEU:HB2	1:A:567:ARG:CD	2.44	0.47
1:A:598:ALA:HA	1:A:601:ARG:HD3	1.97	0.47
1:B:930:LEU:HD13	1:B:950:ARG:HB2	1.97	0.47
1:C:383:ILE:C	1:C:383:ILE:HD12	2.40	0.47
1:D:870:PHE:CD1	1:D:922:TYR:HD2	2.32	0.47
1:D:1056:ILE:HD12	1:D:1216:TYR:CD1	2.49	0.47
1:D:1249:ILE:N	1:D:1250:PRO:CD	2.78	0.47
1:A:271:VAL:O	1:A:275:ILE:HG23	2.15	0.46
1:B:387:PHE:CD1	1:B:447:ARG:CZ	2.99	0.46
1:B:918:VAL:HG21	1:B:929:PHE:CE2	2.49	0.46
1:C:1080:VAL:O	1:C:1080:VAL:HG12	2.14	0.46
1:D:581:THR:HB	1:D:585:GLU:HG3	1.96	0.46
1:D:623:MET:HE1	1:D:673:CYS:CB	2.39	0.46
1:A:170:PRO:HG2	1:A:173:TYR:HD1	1.79	0.46
1:A:581:THR:HB	1:A:585:GLU:HG3	1.97	0.46
1:A:1002:MET:HG3	1:A:1031:LEU:HD11	1.97	0.46
1:B:664:ASP:HB2	1:B:803:LEU:HD11	1.98	0.46
1:B:1145:PHE:HD2	1:B:1146:PHE:CD1	2.33	0.46
1:A:69:TYR:CE2	1:A:97:VAL:HG23	2.51	0.46
1:A:713:ILE:O	1:A:714:LYS:CG	2.53	0.46
1:A:870:PHE:CD1	1:A:922:TYR:HD2	2.31	0.46
1:A:922:TYR:N	1:A:922:TYR:CD1	2.83	0.46
1:B:99:HIS:O	1:B:101:PRO:CD	2.64	0.46
1:B:226:ARG:HH12	1:B:282:ASP:CG	2.24	0.46
1:B:598:ALA:HA	1:B:601:ARG:HD3	1.96	0.46
1:B:664:ASP:HB2	1:B:803:LEU:HD12	1.97	0.46
1:C:262:ASP:O	1:C:266:HIS:ND1	2.44	0.46
1:C:339:LYS:HA	1:C:339:LYS:HD2	1.67	0.46
1:A:376:ASP:CB	1:B:570:VAL:HG21	2.32	0.46
1:A:594:LEU:HG	1:A:604:LEU:HD23	1.96	0.46
1:A:1054:GLY:O	1:A:1055:ASP:CB	2.59	0.46
1:C:174:MET:HA	1:C:177:LEU:HB2	1.97	0.46
1:C:225:SER:O	1:C:226:ARG:C	2.57	0.46
1:C:226:ARG:H	1:C:226:ARG:HG2	1.54	0.46
1:D:150:ASP:O	1:D:151:LEU:HD23	2.16	0.46
1:D:760:SER:HB2	1:D:766:LYS:HZ1	1.80	0.46
1:A:150:ASP:O	1:A:151:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:LEU:CD2	1:A:915:PHE:HE1	2.28	0.46
1:C:359:CYS:SG	1:C:361:SER:HB2	2.55	0.46
1:C:448:VAL:HA	1:C:456:ILE:CD1	2.43	0.46
1:A:441:LEU:HD13	1:A:474:LEU:HD22	1.98	0.46
1:A:574:TYR:N	1:A:574:TYR:CD2	2.77	0.46
1:B:322:PHE:O	1:B:326:VAL:HG23	2.15	0.46
1:B:549:LEU:O	1:B:549:LEU:HG	2.16	0.46
1:C:594:LEU:HG	1:C:604:LEU:HD23	1.96	0.46
1:D:109:ALA:O	1:D:113:VAL:HG23	2.16	0.46
1:D:474:LEU:O	1:D:475:GLN:C	2.57	0.46
1:A:226:ARG:HH12	1:A:282:ASP:CG	2.24	0.46
1:A:230:LEU:HD21	1:A:285:LEU:HD21	1.98	0.46
1:A:316:LEU:O	1:A:316:LEU:HD22	2.15	0.46
1:B:174:MET:HA	1:B:177:LEU:HB2	1.97	0.46
1:B:316:LEU:O	1:B:316:LEU:HD22	2.16	0.46
1:B:440:ILE:O	1:B:444:VAL:HG23	2.16	0.46
1:C:598:ALA:HA	1:C:601:ARG:HD3	1.97	0.46
1:C:623:MET:HE1	1:C:673:CYS:CB	2.40	0.46
1:D:918:VAL:HG21	1:D:929:PHE:CE2	2.50	0.46
1:D:1053:LEU:HD11	1:D:1077:ALA:HA	1.98	0.46
1:A:852:LEU:HD13	1:A:858:VAL:HG23	1.98	0.46
1:B:399:LEU:HD13	1:B:453:SER:O	2.16	0.46
1:C:529:LEU:HA	1:C:532:ARG:NH2	2.31	0.46
1:C:973:PHE:HD1	1:C:974:ASN:H	1.57	0.46
1:C:985:LEU:HB3	1:C:1002:MET:HE1	1.96	0.46
1:D:982:ILE:HD11	1:D:1024:LEU:HG	1.98	0.46
1:B:158:ARG:O	1:B:162:ASP:HB2	2.16	0.46
1:B:911:LEU:CD2	1:B:915:PHE:HE1	2.28	0.46
1:B:1249:ILE:N	1:B:1250:PRO:CD	2.79	0.46
1:C:94:MET:HG2	1:C:132:ILE:CD1	2.45	0.46
1:C:259:ALA:CB	1:C:260:PRO:CD	2.91	0.46
1:C:316:LEU:O	1:C:316:LEU:HD22	2.16	0.46
1:D:298:GLN:HE21	1:D:336:LYS:CG	2.29	0.46
1:D:852:LEU:HD13	1:D:858:VAL:HG23	1.98	0.46
1:D:922:TYR:N	1:D:922:TYR:CD1	2.83	0.46
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.16	0.46
1:B:431:LYS:HG2	1:B:469:TYR:CE1	2.51	0.46
1:B:1164:LEU:HD22	1:B:1252:LEU:CD1	2.46	0.46
1:C:298:GLN:HE21	1:C:336:LYS:CG	2.28	0.46
1:C:922:TYR:N	1:C:922:TYR:HD1	2.14	0.46
1:D:536:VAL:HG11	1:D:603:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:ILE:HG22	1:D:752:LEU:HD11	1.98	0.46
1:D:801:ASP:N	1:D:801:ASP:OD1	2.47	0.46
1:A:109:ALA:O	1:A:113:VAL:HG23	2.16	0.45
1:A:266:HIS:CE1	1:A:373:HIS:HB3	2.51	0.45
1:A:978:ALA:HB1	1:A:1020:PHE:CE1	2.51	0.45
1:A:1056:ILE:HB	1:A:1216:TYR:CZ	2.50	0.45
1:B:430:PHE:CZ	1:B:466:ILE:HG23	2.52	0.45
1:B:774:PHE:HE2	1:B:836:GLU:HG3	1.81	0.45
1:B:1144:THR:O	1:B:1148:GLU:HG2	2.16	0.45
1:C:59:GLU:O	1:C:63:LEU:HG	2.16	0.45
1:C:441:LEU:HD13	1:C:474:LEU:HD22	1.98	0.45
1:D:979:LEU:HD11	1:D:1019:SER:HB2	1.97	0.45
1:A:259:ALA:CB	1:A:260:PRO:CD	2.91	0.45
1:A:667:LEU:HD23	1:A:667:LEU:HA	1.80	0.45
1:B:69:TYR:CE2	1:B:97:VAL:HG23	2.51	0.45
1:B:474:LEU:O	1:B:475:GLN:C	2.57	0.45
1:D:549:LEU:O	1:D:549:LEU:HG	2.16	0.45
1:D:766:LYS:HB2	1:D:766:LYS:HZ2	1.80	0.45
1:A:158:ARG:O	1:A:162:ASP:HB2	2.16	0.45
1:B:227:ARG:NH2	1:B:291:LYS:HD3	2.31	0.45
1:B:230:LEU:HD22	1:B:275:ILE:HD12	1.99	0.45
1:B:238:ARG:NH2	1:B:304:CYS:O	2.50	0.45
1:C:911:LEU:CD2	1:C:915:PHE:HE1	2.29	0.45
1:C:1144:THR:O	1:C:1148:GLU:HG2	2.17	0.45
1:C:1154:LEU:CD1	1:C:1163:LEU:HD12	2.45	0.45
1:D:431:LYS:HG2	1:D:469:TYR:CE1	2.52	0.45
1:D:1144:THR:O	1:D:1148:GLU:HG2	2.16	0.45
1:A:474:LEU:HB3	1:A:477:CYS:SG	2.57	0.45
1:B:1053:LEU:HD11	1:B:1077:ALA:HA	1.99	0.45
1:C:675:ALA:O	1:C:679:SER:HB3	2.17	0.45
1:D:644:LEU:HD21	1:D:708:ILE:HD13	1.98	0.45
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.99	0.45
1:B:109:ALA:O	1:B:113:VAL:HG23	2.16	0.45
1:B:360:VAL:O	1:B:364:ILE:HG13	2.16	0.45
1:B:524:MET:HB3	1:B:592:ARG:HH21	1.80	0.45
1:B:594:LEU:HG	1:B:604:LEU:HD23	1.97	0.45
1:C:266:HIS:CE1	1:C:373:HIS:HB3	2.51	0.45
1:C:372:VAL:HG22	1:C:432:ILE:CG2	2.46	0.45
1:C:573:ARG:NH2	1:D:323:GLU:OE2	2.50	0.45
1:C:671:GLN:OE1	1:C:672:HIS:CD2	2.70	0.45
1:D:360:VAL:O	1:D:364:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:675:ALA:O	1:D:679:SER:HB3	2.17	0.45
1:A:529:LEU:HD21	1:A:600:ILE:HG13	1.99	0.45
1:A:671:GLN:OE1	1:A:671:GLN:C	2.60	0.45
1:A:826:GLU:HA	1:A:829:SER:HG	1.81	0.45
1:A:979:LEU:HD11	1:A:1019:SER:HB2	1.99	0.45
1:B:297:GLN:H	1:B:297:GLN:HG2	1.60	0.45
1:B:644:LEU:HD21	1:B:708:ILE:HD13	1.98	0.45
1:C:109:ALA:O	1:C:113:VAL:HG23	2.16	0.45
1:C:217:LEU:CD2	1:C:229:VAL:HG13	2.43	0.45
1:C:271:VAL:O	1:C:275:ILE:HG23	2.16	0.45
1:C:277:PHE:CZ	1:D:551:SER:C	2.93	0.45
1:C:881:LEU:HG	1:C:911:LEU:HD21	1.99	0.45
1:D:524:MET:HB3	1:D:592:ARG:HH21	1.81	0.45
1:D:881:LEU:HG	1:D:911:LEU:HD21	1.99	0.45
1:A:59:GLU:O	1:A:63:LEU:HG	2.16	0.45
1:A:476:ASN:N	1:A:476:ASN:OD1	2.50	0.45
1:A:881:LEU:HG	1:A:911:LEU:HD21	1.98	0.45
1:A:922:TYR:N	1:A:922:TYR:HD1	2.15	0.45
1:B:922:TYR:N	1:B:922:TYR:HD1	2.15	0.45
1:C:430:PHE:CZ	1:C:466:ILE:HG23	2.52	0.45
1:D:158:ARG:O	1:D:162:ASP:HB2	2.16	0.45
1:D:174:MET:HA	1:D:177:LEU:HB2	1.97	0.45
1:D:368:VAL:HG11	1:D:428:GLU:HB3	1.98	0.45
1:A:151:LEU:HD12	1:A:156:TYR:CZ	2.52	0.45
1:B:672:HIS:HE1	1:B:805:SER:HB3	1.81	0.45
1:C:1249:ILE:N	1:C:1250:PRO:CD	2.79	0.45
1:D:1174:LEU:O	1:D:1178:VAL:HG23	2.17	0.45
1:A:360:VAL:O	1:A:364:ILE:HG13	2.16	0.45
1:A:376:ASP:HB2	1:B:570:VAL:CG2	2.30	0.45
1:A:474:LEU:O	1:A:475:GLN:C	2.57	0.45
1:A:1260:GLU:HA	1:A:1263:LEU:HD12	1.99	0.45
1:B:150:ASP:O	1:B:151:LEU:HD23	2.17	0.45
1:B:266:HIS:CE1	1:B:373:HIS:HB3	2.51	0.45
1:B:706:GLU:O	1:B:709:THR:HB	2.17	0.45
1:C:226:ARG:HH12	1:C:282:ASP:CG	2.25	0.45
1:C:508:ILE:O	1:D:435:MET:HG3	2.16	0.45
1:C:540:LEU:O	1:C:544:LYS:HG3	2.17	0.45
1:D:713:ILE:CG2	1:D:772:SER:HB3	2.46	0.45
1:A:149:GLY:C	1:A:151:LEU:H	2.24	0.45
1:B:271:VAL:O	1:B:275:ILE:HG23	2.15	0.45
1:B:852:LEU:HD13	1:B:858:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:GLN:HG2	1:C:60:ASP:OD2	2.18	0.45
1:C:474:LEU:O	1:C:475:GLN:C	2.57	0.45
1:C:1174:LEU:O	1:C:1178:VAL:HG23	2.17	0.45
1:D:266:HIS:CE1	1:D:373:HIS:HB3	2.51	0.45
1:A:349:PHE:O	1:A:353:LEU:HG	2.17	0.44
1:A:945:VAL:O	1:A:949:GLN:HB2	2.17	0.44
1:A:996:SER:HB3	1:A:999:PHE:CB	2.47	0.44
1:B:344:LEU:HD23	1:B:350:LEU:HB3	1.99	0.44
1:B:801:ASP:N	1:B:801:ASP:OD1	2.48	0.44
1:B:1150:VAL:O	1:B:1213:PHE:HD1	2.00	0.44
1:C:158:ARG:O	1:C:162:ASP:HB2	2.16	0.44
1:C:1056:ILE:HD12	1:C:1216:TYR:CD1	2.53	0.44
1:D:349:PHE:O	1:D:353:LEU:HG	2.17	0.44
1:D:474:LEU:HB3	1:D:477:CYS:SG	2.56	0.44
1:A:430:PHE:CZ	1:A:466:ILE:HG23	2.53	0.44
1:A:573:ARG:NH2	1:B:323:GLU:OE2	2.51	0.44
1:A:973:PHE:CD1	1:A:974:ASN:N	2.72	0.44
1:A:1249:ILE:N	1:A:1250:PRO:CD	2.79	0.44
1:B:259:ALA:CB	1:B:260:PRO:CD	2.91	0.44
1:B:945:VAL:O	1:B:949:GLN:HB2	2.17	0.44
1:B:1154:LEU:CD1	1:B:1163:LEU:HD12	2.45	0.44
1:C:41:ARG:N	1:C:41:ARG:HD3	2.32	0.44
1:C:51:LEU:HD13	1:C:96:GLU:HG2	1.98	0.44
1:C:644:LEU:HD21	1:C:708:ILE:HD13	1.98	0.44
1:C:671:GLN:OE1	1:C:671:GLN:C	2.59	0.44
1:C:1260:GLU:HA	1:C:1263:LEU:HD12	2.00	0.44
1:D:383:ILE:C	1:D:383:ILE:HD12	2.43	0.44
1:D:441:LEU:HD13	1:D:474:LEU:HD22	1.99	0.44
1:D:476:ASN:N	1:D:476:ASN:OD1	2.50	0.44
1:D:671:GLN:OE1	1:D:671:GLN:C	2.61	0.44
1:D:945:VAL:O	1:D:949:GLN:HB2	2.17	0.44
1:A:344:LEU:HD23	1:A:350:LEU:HB3	1.99	0.44
1:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.98	0.44
1:B:441:LEU:HD13	1:B:474:LEU:HD22	1.99	0.44
1:C:513:ARG:NH1	1:C:514:ASP:OD1	2.51	0.44
1:C:852:LEU:HD13	1:C:858:VAL:HG23	1.98	0.44
1:A:548:VAL:O	1:A:569:ASP:HB3	2.17	0.44
1:A:672:HIS:CE1	1:A:861:PRO:HG3	2.52	0.44
1:B:149:GLY:C	1:B:151:LEU:H	2.23	0.44
1:B:476:ASN:N	1:B:476:ASN:OD1	2.50	0.44
1:B:996:SER:HB3	1:B:999:PHE:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HD23	1:C:350:LEU:HB3	2.00	0.44
1:C:349:PHE:O	1:C:353:LEU:HG	2.17	0.44
1:A:211:PRO:N	1:A:212:PRO:HD2	2.33	0.44
1:A:217:LEU:O	1:A:217:LEU:HD23	2.17	0.44
1:A:529:LEU:HA	1:A:532:ARG:NH2	2.33	0.44
1:B:519:VAL:HG12	1:B:520:LEU:N	2.32	0.44
1:C:69:TYR:CE2	1:C:97:VAL:HG23	2.51	0.44
1:C:217:LEU:HD22	1:C:229:VAL:CG1	2.42	0.44
1:C:1053:LEU:HD11	1:C:1077:ALA:HA	1.99	0.44
1:C:1077:ALA:CB	1:C:1078:PRO:HD3	2.40	0.44
1:D:297:GLN:HG3	1:D:1104:GLY:CA	2.47	0.44
1:D:387:PHE:CD1	1:D:447:ARG:CZ	3.01	0.44
1:D:563:VAL:O	1:D:563:VAL:HG13	2.17	0.44
1:D:973:PHE:HD1	1:D:974:ASN:H	1.57	0.44
1:A:217:LEU:CD2	1:A:229:VAL:HG13	2.41	0.44
1:A:519:VAL:HG12	1:A:520:LEU:N	2.32	0.44
1:B:151:LEU:HD12	1:B:156:TYR:CZ	2.53	0.44
1:B:217:LEU:HD23	1:B:217:LEU:O	2.17	0.44
1:B:474:LEU:HB3	1:B:477:CYS:SG	2.57	0.44
1:B:604:LEU:HG	1:B:608:PHE:CE1	2.52	0.44
1:C:476:ASN:N	1:C:476:ASN:OD1	2.50	0.44
1:C:574:TYR:CD1	1:D:439:GLU:HG2	2.53	0.44
1:C:671:GLN:CG	1:C:755:TYR:HB2	2.47	0.44
1:D:989:SER:HB2	1:D:1031:LEU:HD21	2.00	0.44
1:A:221:SER:O	1:A:224:GLY:N	2.51	0.44
1:A:540:LEU:O	1:A:544:LYS:HG3	2.17	0.44
1:A:1174:LEU:O	1:A:1178:VAL:HG23	2.17	0.44
1:B:211:PRO:N	1:B:212:PRO:HD2	2.33	0.44
1:B:548:VAL:CG1	1:B:580:GLU:HA	2.48	0.44
1:B:838:MET:HA	1:B:838:MET:CE	2.42	0.44
1:C:15:ASP:OD1	1:C:15:ASP:N	2.47	0.44
1:C:396:LYS:HE2	1:C:396:LYS:HB3	1.90	0.44
1:C:996:SER:HB3	1:C:999:PHE:CB	2.48	0.44
1:C:1002:MET:HG3	1:C:1031:LEU:CD1	2.47	0.44
1:D:151:LEU:HD12	1:D:156:TYR:CZ	2.53	0.44
1:D:193:LEU:O	1:D:197:LYS:HG2	2.18	0.44
1:D:211:PRO:N	1:D:212:PRO:HD2	2.33	0.44
1:D:344:LEU:HD23	1:D:350:LEU:HB3	1.99	0.44
1:D:430:PHE:CZ	1:D:466:ILE:HG23	2.52	0.44
1:D:1046:SER:HB2	1:D:1148:GLU:HB2	2.00	0.44
1:A:22:GLN:HG2	1:A:60:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:VAL:HG13	1:A:657:ILE:HG23	2.00	0.44
1:A:675:ALA:O	1:A:679:SER:HB3	2.17	0.44
1:B:298:GLN:HE21	1:B:336:LYS:CG	2.28	0.44
1:B:1049:ILE:H	1:B:1049:ILE:HG13	1.57	0.44
1:C:221:SER:O	1:C:224:GLY:N	2.51	0.44
1:C:341:LEU:HD11	1:C:359:CYS:HB3	2.00	0.44
1:D:120:ARG:HG2	1:D:172:ARG:HH12	1.82	0.44
1:D:604:LEU:HG	1:D:608:PHE:CE1	2.53	0.44
1:A:41:ARG:N	1:A:41:ARG:HD3	2.33	0.44
1:A:90:ILE:O	1:A:94:MET:HG3	2.18	0.44
1:A:447:ARG:O	1:A:456:ILE:HD11	2.18	0.44
1:A:510:MET:HG2	1:B:435:MET:HE2	1.99	0.44
1:A:1049:ILE:H	1:A:1049:ILE:HG13	1.57	0.44
1:B:529:LEU:HA	1:B:532:ARG:NH2	2.32	0.44
1:B:667:LEU:HD23	1:B:667:LEU:HA	1.80	0.44
1:C:335:VAL:HG13	1:C:414:THR:CG2	2.46	0.44
1:C:431:LYS:HG2	1:C:469:TYR:CE1	2.53	0.44
1:D:242:LYS:HA	1:D:245:ARG:HE	1.83	0.44
1:D:529:LEU:HD22	1:D:533:LYS:HE3	1.99	0.44
1:D:529:LEU:HA	1:D:532:ARG:NH2	2.33	0.44
1:D:706:GLU:O	1:D:709:THR:HB	2.18	0.44
1:A:297:GLN:H	1:A:297:GLN:HG2	1.62	0.43
1:B:389:LEU:HD13	1:B:421:LEU:HD23	2.00	0.43
1:B:549:LEU:HD23	1:B:569:ASP:OD1	2.18	0.43
1:B:634:TYR:CG	1:B:704:MET:HE3	2.53	0.43
1:B:675:ALA:O	1:B:679:SER:HB3	2.17	0.43
1:C:211:PRO:N	1:C:212:PRO:HD2	2.33	0.43
1:C:540:LEU:CD1	1:C:607:GLY:HA3	2.48	0.43
1:C:1046:SER:HB2	1:C:1148:GLU:HB2	2.00	0.43
1:D:519:VAL:HG12	1:D:520:LEU:N	2.32	0.43
1:D:672:HIS:CE1	1:D:805:SER:HB3	2.53	0.43
1:A:664:ASP:O	1:A:751:VAL:HG21	2.18	0.43
1:B:563:VAL:O	1:B:563:VAL:HG13	2.17	0.43
1:B:860:GLY:HA3	1:B:861:PRO:HD2	1.76	0.43
1:C:563:VAL:O	1:C:563:VAL:HG13	2.17	0.43
1:C:978:ALA:HB1	1:C:1020:PHE:CE1	2.53	0.43
1:C:1164:LEU:HD22	1:C:1252:LEU:CD1	2.48	0.43
1:D:540:LEU:O	1:D:544:LYS:HG3	2.18	0.43
1:A:431:LYS:HG2	1:A:469:TYR:CE1	2.53	0.43
1:A:619:ALA:O	1:A:623:MET:HB2	2.19	0.43
1:A:821:ILE:H	1:A:821:ILE:HG13	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LEU:O	1:B:197:LYS:HG2	2.18	0.43
1:B:540:LEU:O	1:B:544:LYS:HG3	2.18	0.43
1:C:193:LEU:O	1:C:197:LYS:HG2	2.18	0.43
1:C:439:GLU:HG2	1:D:574:TYR:CZ	2.54	0.43
1:C:619:ALA:O	1:C:623:MET:HB2	2.18	0.43
1:C:650:VAL:HG13	1:C:657:ILE:HG23	2.00	0.43
1:C:708:ILE:HG22	1:C:752:LEU:HD11	1.99	0.43
1:C:945:VAL:O	1:C:949:GLN:HB2	2.17	0.43
1:C:952:SER:HB3	1:C:998:GLN:HB3	2.01	0.43
1:C:1145:PHE:CD2	1:C:1146:PHE:CD1	3.07	0.43
1:C:1270:SER:OG	1:C:1271:LYS:N	2.51	0.43
1:D:1260:GLU:HA	1:D:1263:LEU:HD12	1.99	0.43
1:A:563:VAL:O	1:A:563:VAL:HG13	2.17	0.43
1:B:881:LEU:HG	1:B:911:LEU:HD21	1.99	0.43
1:B:1050:HIS:HA	1:B:1152:THR:OG1	2.18	0.43
1:C:151:LEU:HD12	1:C:156:TYR:CZ	2.52	0.43
1:C:283:CYS:O	1:C:287:ARG:HG3	2.18	0.43
1:C:323:GLU:OE2	1:D:573:ARG:NH2	2.51	0.43
1:C:474:LEU:HB3	1:C:477:CYS:SG	2.59	0.43
1:C:667:LEU:HB3	1:C:751:VAL:HG11	2.00	0.43
1:D:922:TYR:N	1:D:922:TYR:HD1	2.14	0.43
1:A:185:CYS:O	1:A:186:LEU:HD23	2.19	0.43
1:A:816:LEU:CD1	1:A:838:MET:HE1	2.39	0.43
1:B:1260:GLU:HA	1:B:1263:LEU:HD12	1.99	0.43
1:C:466:ILE:O	1:C:469:TYR:HB3	2.18	0.43
1:D:339:LYS:HA	1:D:339:LYS:HD2	1.66	0.43
1:D:382:LEU:HD22	1:D:425:ILE:HG23	2.00	0.43
1:D:502:VAL:O	1:D:502:VAL:HG13	2.18	0.43
1:D:996:SER:HB3	1:D:999:PHE:CB	2.48	0.43
1:A:121:LEU:C	1:A:123:ASN:N	2.68	0.43
1:A:1003:LEU:HG	1:A:1031:LEU:HB3	2.01	0.43
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.45	0.43
1:B:694:GLU:O	1:B:698:TYR:HD1	2.02	0.43
1:B:1174:LEU:O	1:B:1178:VAL:HG23	2.18	0.43
1:C:957:GLN:HG3	1:C:960:ARG:NH2	2.34	0.43
1:D:623:MET:HE3	1:D:698:TYR:OH	2.18	0.43
1:A:995:THR:HB	1:A:996:SER:H	1.66	0.43
1:B:242:LYS:HA	1:B:245:ARG:HE	1.83	0.43
1:B:383:ILE:C	1:B:383:ILE:HD12	2.44	0.43
1:B:466:ILE:O	1:B:469:TYR:HB3	2.19	0.43
1:C:382:LEU:HD22	1:C:425:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:VAL:O	1:C:502:VAL:HG13	2.19	0.43
1:C:524:MET:CB	1:C:592:ARG:HH21	2.31	0.43
1:D:657:ILE:HD12	1:D:733:ASN:O	2.17	0.43
1:A:283:CYS:O	1:A:287:ARG:HG3	2.18	0.43
1:A:341:LEU:HD11	1:A:359:CYS:HB3	2.01	0.43
1:A:1143:VAL:HG13	1:A:1206:LEU:HG	1.99	0.43
1:B:952:SER:HB3	1:B:998:GLN:HB3	2.01	0.43
1:B:954:GLN:O	1:B:958:PHE:HD1	2.02	0.43
1:C:217:LEU:HD23	1:C:217:LEU:O	2.18	0.43
1:C:549:LEU:O	1:C:549:LEU:HG	2.18	0.43
1:D:447:ARG:O	1:D:456:ILE:HD11	2.19	0.43
1:D:650:VAL:HG13	1:D:657:ILE:HG23	2.00	0.43
1:D:804:LEU:O	1:D:848:LYS:NZ	2.51	0.43
1:A:298:GLN:HE21	1:A:336:LYS:CG	2.29	0.43
1:A:383:ILE:HG13	1:A:384:GLU:N	2.34	0.43
1:A:549:LEU:O	1:A:549:LEU:HG	2.19	0.43
1:A:804:LEU:O	1:A:848:LYS:NZ	2.51	0.43
1:A:952:SER:HB3	1:A:998:GLN:HB3	2.01	0.43
1:B:383:ILE:HG13	1:B:384:GLU:N	2.34	0.43
1:B:762:PHE:CD1	1:B:762:PHE:N	2.86	0.43
1:B:804:LEU:O	1:B:848:LYS:NZ	2.50	0.43
1:C:1156:SER:HA	1:C:1160:VAL:HG21	2.01	0.43
1:D:221:SER:O	1:D:224:GLY:N	2.51	0.43
1:A:227:ARG:HG3	1:A:288:GLU:HG3	2.00	0.43
1:A:466:ILE:O	1:A:469:TYR:HB3	2.19	0.43
1:A:508:ILE:O	1:B:435:MET:HG3	2.18	0.43
1:A:549:LEU:HB2	1:A:567:ARG:HD2	2.01	0.43
1:A:1156:SER:HA	1:A:1160:VAL:HG21	2.01	0.43
1:A:1199:VAL:O	1:A:1202:SER:OG	2.30	0.43
1:B:349:PHE:O	1:B:353:LEU:HG	2.17	0.43
1:B:385:PHE:CE2	1:B:389:LEU:HD11	2.54	0.43
1:B:387:PHE:CZ	1:B:443:GLN:HB3	2.53	0.43
1:B:973:PHE:CD1	1:B:974:ASN:N	2.72	0.43
1:C:801:ASP:OD1	1:C:801:ASP:N	2.47	0.43
1:C:880:LEU:HD22	1:C:907:CYS:HA	2.01	0.43
1:D:694:GLU:O	1:D:698:TYR:HD1	2.02	0.43
1:D:952:SER:HB3	1:D:998:GLN:HB3	2.00	0.43
1:B:1145:PHE:CD2	1:B:1146:PHE:CD1	3.07	0.42
1:C:297:GLN:H	1:C:297:GLN:HG2	1.62	0.42
1:C:623:MET:HE3	1:C:698:TYR:OH	2.19	0.42
1:D:165:CYS:HB3	1:D:197:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:PHE:CZ	1:D:443:GLN:HB3	2.54	0.42
1:D:1185:CYS:SG	1:D:1191:ILE:HG12	2.59	0.42
1:A:193:LEU:O	1:A:197:LYS:HG2	2.19	0.42
1:A:513:ARG:NH1	1:A:514:ASP:OD1	2.52	0.42
1:A:634:TYR:CG	1:A:704:MET:HE3	2.54	0.42
1:A:1005:TRP:O	1:A:1009:ILE:HG13	2.19	0.42
1:B:165:CYS:HB3	1:B:197:LYS:HE3	2.01	0.42
1:B:221:SER:O	1:B:224:GLY:N	2.52	0.42
1:B:708:ILE:HG22	1:B:752:LEU:HD11	2.01	0.42
1:B:885:THR:O	1:B:886:SER:HB2	2.19	0.42
1:C:185:CYS:O	1:C:186:LEU:HD23	2.19	0.42
1:C:456:ILE:O	1:C:456:ILE:CG2	2.67	0.42
1:C:529:LEU:HD21	1:C:600:ILE:HG13	2.02	0.42
1:D:885:THR:O	1:D:886:SER:HB2	2.19	0.42
1:D:954:GLN:O	1:D:958:PHE:HD1	2.02	0.42
1:A:120:ARG:HG2	1:A:172:ARG:HH12	1.82	0.42
1:A:706:GLU:O	1:A:709:THR:HB	2.19	0.42
1:B:957:GLN:HG3	1:B:960:ARG:NH2	2.33	0.42
1:C:165:CYS:HB3	1:C:197:LYS:HE3	2.01	0.42
1:C:635:GLU:O	1:C:711:ARG:NH2	2.40	0.42
1:C:1182:LEU:O	1:C:1186:GLN:HG3	2.19	0.42
1:D:217:LEU:HD22	1:D:229:VAL:CG1	2.43	0.42
1:D:335:VAL:HG13	1:D:414:THR:HG21	2.00	0.42
1:D:349:PHE:CD2	1:D:1037:SER:HB3	2.54	0.42
1:A:524:MET:HB3	1:A:592:ARG:HH21	1.83	0.42
1:A:573:ARG:HE	1:A:573:ARG:HB2	1.70	0.42
1:A:694:GLU:O	1:A:698:TYR:HD1	2.03	0.42
1:B:227:ARG:HH21	1:B:291:LYS:CD	2.32	0.42
1:B:619:ALA:O	1:B:623:MET:HB2	2.18	0.42
1:C:90:ILE:CD1	1:C:125:LYS:HB3	2.49	0.42
1:C:440:ILE:O	1:C:444:VAL:HG23	2.18	0.42
1:C:885:THR:O	1:C:886:SER:HB2	2.20	0.42
1:C:1199:VAL:O	1:C:1202:SER:OG	2.30	0.42
1:D:185:CYS:O	1:D:186:LEU:HD23	2.19	0.42
1:D:440:ILE:O	1:D:444:VAL:HG23	2.19	0.42
1:A:165:CYS:HB3	1:A:197:LYS:HE3	2.01	0.42
1:A:927:GLN:HG2	1:A:947:VAL:HG22	2.00	0.42
1:B:185:CYS:O	1:B:186:LEU:HD23	2.19	0.42
1:B:329:LEU:HD12	1:B:329:LEU:O	2.20	0.42
1:C:3:LEU:HD23	1:C:6:LEU:HD12	2.01	0.42
1:C:60:ASP:O	1:C:64:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:HD3	1:C:100:PHE:CZ	2.55	0.42
1:C:242:LYS:HA	1:C:245:ARG:HE	1.84	0.42
1:C:706:GLU:O	1:C:709:THR:HB	2.19	0.42
1:D:396:LYS:HE2	1:D:396:LYS:HB3	1.90	0.42
1:D:473:ILE:HG13	1:D:473:ILE:H	1.61	0.42
1:D:634:TYR:CG	1:D:704:MET:HE3	2.54	0.42
1:D:762:PHE:N	1:D:762:PHE:CD1	2.86	0.42
1:D:1145:PHE:CD2	1:D:1146:PHE:CD1	3.07	0.42
1:A:66:TYR:CD1	1:A:104:LEU:HD22	2.54	0.42
1:A:242:LYS:HA	1:A:245:ARG:HE	1.84	0.42
1:A:474:LEU:HD22	1:A:477:CYS:SG	2.59	0.42
1:A:954:GLN:O	1:A:958:PHE:HD1	2.03	0.42
1:A:957:GLN:HG3	1:A:960:ARG:NH2	2.34	0.42
1:B:1185:CYS:SG	1:B:1191:ILE:HG12	2.59	0.42
1:B:1270:SER:OG	1:B:1271:LYS:N	2.52	0.42
1:C:762:PHE:CD1	1:C:762:PHE:N	2.87	0.42
1:C:954:GLN:O	1:C:958:PHE:HD1	2.03	0.42
1:D:966:LEU:HB3	1:D:1013:TYR:CZ	2.54	0.42
1:A:1103:LYS:HE2	1:A:1103:LYS:HB3	1.79	0.42
1:A:1145:PHE:CD2	1:A:1146:PHE:CD1	3.07	0.42
1:B:502:VAL:O	1:B:502:VAL:HG13	2.19	0.42
1:B:529:LEU:HD22	1:B:533:LYS:HE3	2.00	0.42
1:B:650:VAL:HG13	1:B:657:ILE:HG23	2.00	0.42
1:B:1077:ALA:CB	1:B:1078:PRO:HD3	2.40	0.42
1:B:1103:LYS:HE2	1:B:1103:LYS:HB3	1.80	0.42
1:C:120:ARG:HG2	1:C:172:ARG:HH12	1.82	0.42
1:C:474:LEU:HD22	1:C:477:CYS:SG	2.59	0.42
1:C:634:TYR:CG	1:C:704:MET:HE3	2.54	0.42
1:C:694:GLU:O	1:C:698:TYR:HD1	2.03	0.42
1:C:1005:TRP:O	1:C:1009:ILE:HG13	2.19	0.42
1:D:283:CYS:O	1:D:287:ARG:HG3	2.20	0.42
1:D:880:LEU:HD22	1:D:907:CYS:HA	2.02	0.42
1:D:957:GLN:HG3	1:D:960:ARG:NH2	2.34	0.42
1:D:1182:LEU:O	1:D:1186:GLN:HG3	2.19	0.42
1:A:244:HIS:CD2	1:A:260:PRO:HG2	2.54	0.42
1:A:529:LEU:HD22	1:A:533:LYS:HE3	2.00	0.42
1:A:762:PHE:CD1	1:A:762:PHE:N	2.87	0.42
1:A:1071:VAL:HG12	1:A:1075:THR:HG21	2.02	0.42
1:B:77:GLU:CB	1:B:121:LEU:HA	2.31	0.42
1:B:329:LEU:HD12	1:B:329:LEU:C	2.45	0.42
1:B:353:LEU:HB3	1:B:1131:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:TRP:O	1:B:1009:ILE:HG13	2.19	0.42
1:C:519:VAL:HG12	1:C:520:LEU:N	2.34	0.42
1:D:149:GLY:C	1:D:151:LEU:H	2.24	0.42
1:D:597:GLN:H	1:D:597:GLN:HG2	1.50	0.42
1:A:3:LEU:HD23	1:A:6:LEU:HD12	2.01	0.42
1:A:1053:LEU:HD23	1:A:1053:LEU:HA	1.86	0.42
1:A:1136:VAL:HG11	1:A:1194:THR:HG22	2.02	0.42
1:B:113:VAL:HG22	1:B:164:LEU:HG	2.01	0.42
1:B:217:LEU:HD22	1:B:229:VAL:CG1	2.44	0.42
1:B:661:GLU:HA	1:B:662:PRO:HD2	1.92	0.42
1:B:1156:SER:HA	1:B:1160:VAL:HG21	2.01	0.42
1:C:1158:SER:O	1:C:1161:ASP:N	2.53	0.42
1:D:763:SER:O	1:D:767:PHE:CD1	2.72	0.42
1:D:1156:SER:HA	1:D:1160:VAL:HG21	2.01	0.42
1:A:766:LYS:HB2	1:A:766:LYS:HZ2	1.84	0.42
1:A:1182:LEU:O	1:A:1186:GLN:HG3	2.19	0.42
1:A:1200:LYS:HB3	1:A:1274:LEU:CD2	2.50	0.42
1:B:1005:TRP:CE2	1:B:1009:ILE:HD11	2.55	0.42
1:C:609:TYR:CE2	1:C:861:PRO:HB3	2.55	0.42
1:C:817:PHE:HB3	1:C:882:TRP:CZ3	2.55	0.42
1:C:995:THR:HB	1:C:996:SER:H	1.66	0.42
1:D:217:LEU:O	1:D:217:LEU:HD23	2.19	0.42
1:D:474:LEU:HD22	1:D:477:CYS:SG	2.60	0.42
1:A:440:ILE:O	1:A:444:VAL:HG23	2.19	0.41
1:A:763:SER:O	1:A:767:PHE:CD1	2.72	0.41
1:A:814:THR:OG1	1:A:879:VAL:HG21	2.20	0.41
1:A:834:SER:OG	1:A:837:PHE:HB3	2.20	0.41
1:A:1042:LEU:O	1:A:1145:PHE:HD1	2.03	0.41
1:B:1158:SER:O	1:B:1161:ASP:N	2.53	0.41
1:C:973:PHE:CD1	1:C:974:ASN:N	2.72	0.41
1:D:113:VAL:HG22	1:D:164:LEU:HG	2.01	0.41
1:D:383:ILE:HG13	1:D:384:GLU:N	2.34	0.41
1:D:466:ILE:O	1:D:469:TYR:HB3	2.19	0.41
1:A:96:GLU:OE1	1:A:96:GLU:HA	2.20	0.41
1:A:169:TRP:CZ3	1:A:177:LEU:HB3	2.56	0.41
1:A:860:GLY:HA3	1:A:861:PRO:HD2	1.77	0.41
1:B:573:ARG:HE	1:B:573:ARG:HB2	1.71	0.41
1:B:623:MET:HE3	1:B:698:TYR:OH	2.19	0.41
1:B:834:SER:OG	1:B:837:PHE:HB3	2.20	0.41
1:B:978:ALA:HB1	1:B:1020:PHE:CE1	2.55	0.41
1:B:1005:TRP:CZ2	1:B:1009:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1182:LEU:O	1:B:1186:GLN:HG3	2.20	0.41
1:C:329:LEU:C	1:C:329:LEU:HD12	2.45	0.41
1:C:368:VAL:HG11	1:C:428:GLU:HB3	2.02	0.41
1:C:447:ARG:O	1:C:456:ILE:HD11	2.19	0.41
1:C:623:MET:HE3	1:C:698:TYR:CE2	2.55	0.41
1:C:763:SER:O	1:C:767:PHE:CD1	2.72	0.41
1:C:1150:VAL:O	1:C:1213:PHE:HD1	2.03	0.41
1:D:127:LEU:HB3	1:D:180:VAL:HG21	2.02	0.41
1:D:297:GLN:HB2	1:D:1104:GLY:HA3	2.02	0.41
1:D:329:LEU:C	1:D:329:LEU:HD12	2.45	0.41
1:D:524:MET:HB2	1:D:592:ARG:HH21	1.85	0.41
1:D:664:ASP:OD1	1:D:664:ASP:N	2.54	0.41
1:D:817:PHE:HB3	1:D:882:TRP:CZ3	2.56	0.41
1:D:1270:SER:OG	1:D:1271:LYS:N	2.52	0.41
1:A:1050:HIS:HB2	1:A:1148:GLU:O	2.20	0.41
1:B:391:ASP:CG	1:B:447:ARG:HH12	2.28	0.41
1:C:12:LYS:HD3	1:C:12:LYS:HA	1.93	0.41
1:C:549:LEU:HD13	1:D:273:LEU:HD21	2.02	0.41
1:A:226:ARG:NH1	1:A:282:ASP:OD1	2.54	0.41
1:A:502:VAL:O	1:A:502:VAL:HG13	2.20	0.41
1:A:533:LYS:HE3	1:A:533:LYS:HB2	1.91	0.41
1:A:928:GLN:H	1:A:928:GLN:HG2	1.59	0.41
1:B:283:CYS:O	1:B:287:ARG:HG3	2.20	0.41
1:B:503:GLN:HG2	1:B:541:LEU:HD21	2.03	0.41
1:C:529:LEU:HD22	1:C:533:LYS:HE3	2.03	0.41
1:C:667:LEU:HD23	1:C:667:LEU:HA	1.79	0.41
1:C:996:SER:HB3	1:C:999:PHE:HB3	2.03	0.41
1:C:1049:ILE:H	1:C:1049:ILE:HG13	1.57	0.41
1:D:341:LEU:HD11	1:D:359:CYS:HB3	2.01	0.41
1:D:548:VAL:CG1	1:D:580:GLU:HA	2.50	0.41
1:D:1005:TRP:CZ2	1:D:1009:ILE:HD11	2.55	0.41
1:D:1092:LEU:HD13	1:D:1169:LYS:HG2	2.01	0.41
1:A:637:GLU:HB3	1:A:640:LEU:HG	2.03	0.41
1:A:817:PHE:HB3	1:A:882:TRP:CZ3	2.55	0.41
1:B:177:LEU:O	1:B:180:VAL:HB	2.20	0.41
1:B:341:LEU:HD11	1:B:359:CYS:HB3	2.01	0.41
1:B:391:ASP:CG	1:B:447:ARG:NH1	2.78	0.41
1:B:536:VAL:HG11	1:B:603:MET:HE3	2.02	0.41
1:C:90:ILE:O	1:C:94:MET:HG3	2.21	0.41
1:C:96:GLU:OE1	1:C:96:GLU:HA	2.20	0.41
1:C:169:TRP:CZ3	1:C:177:LEU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LEU:HD12	1:C:329:LEU:O	2.21	0.41
1:D:141:LYS:O	1:D:142:GLU:HG3	2.20	0.41
1:D:177:LEU:O	1:D:180:VAL:HB	2.21	0.41
1:D:456:ILE:O	1:D:456:ILE:CG2	2.68	0.41
1:D:834:SER:OG	1:D:837:PHE:HB3	2.20	0.41
1:D:1005:TRP:CE2	1:D:1009:ILE:HD11	2.55	0.41
1:D:1005:TRP:O	1:D:1009:ILE:HG13	2.20	0.41
1:A:65:ARG:HD3	1:A:100:PHE:CZ	2.54	0.41
1:A:113:VAL:HG22	1:A:164:LEU:HG	2.03	0.41
1:A:623:MET:HE3	1:A:698:TYR:OH	2.20	0.41
1:A:1046:SER:HB2	1:A:1148:GLU:HB2	2.03	0.41
1:A:1270:SER:OG	1:A:1271:LYS:N	2.52	0.41
1:B:217:LEU:CD2	1:B:229:VAL:HG13	2.45	0.41
1:C:152:ASN:HB2	1:C:154:GLU:HG2	2.03	0.41
1:C:804:LEU:O	1:C:848:LYS:NZ	2.51	0.41
1:D:503:GLN:HG2	1:D:541:LEU:HD21	2.02	0.41
1:D:619:ALA:O	1:D:623:MET:HB2	2.19	0.41
1:D:1158:SER:O	1:D:1161:ASP:N	2.53	0.41
1:A:91:GLY:O	1:A:95:LEU:HG	2.21	0.41
1:A:533:LYS:HG3	1:A:603:MET:HE1	2.02	0.41
1:A:750:GLU:OE2	1:A:802:SER:HA	2.21	0.41
1:A:838:MET:HA	1:A:838:MET:CE	2.42	0.41
1:B:637:GLU:HB3	1:B:640:LEU:HG	2.03	0.41
1:B:672:HIS:CE1	1:B:805:SER:HB3	2.54	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CZ3	2.55	0.41
1:B:880:LEU:HD22	1:B:907:CYS:HA	2.01	0.41
1:C:834:SER:OG	1:C:837:PHE:HB3	2.20	0.41
1:C:1042:LEU:CD2	1:C:1084:VAL:HG12	2.51	0.41
1:C:1249:ILE:H	1:C:1249:ILE:HG13	1.68	0.41
1:D:664:ASP:HB2	1:D:803:LEU:CD1	2.50	0.41
1:D:1103:LYS:HB3	1:D:1103:LYS:HE2	1.79	0.41
1:A:141:LYS:O	1:A:142:GLU:HG3	2.21	0.41
1:A:383:ILE:HD12	1:A:383:ILE:C	2.45	0.41
1:A:1103:LYS:HG2	1:A:1180:TYR:HD1	1.86	0.41
1:B:1053:LEU:HD23	1:B:1053:LEU:HA	1.86	0.41
1:B:1056:ILE:HD12	1:B:1216:TYR:CG	2.56	0.41
1:B:1272:VAL:HG12	1:B:1273:ASN:N	2.36	0.41
1:C:1272:VAL:HG12	1:C:1273:ASN:N	2.36	0.41
1:D:297:GLN:CB	1:D:1104:GLY:HA3	2.50	0.41
1:D:915:PHE:CE2	1:D:988:LEU:HD21	2.56	0.41
1:D:1103:LYS:HG2	1:D:1180:TYR:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HB3	1:A:64:ARG:CZ	2.50	0.41
1:A:95:LEU:HA	1:A:98:HIS:HE1	1.86	0.41
1:A:95:LEU:O	1:A:98:HIS:CE1	2.74	0.41
1:A:329:LEU:HD12	1:A:329:LEU:O	2.21	0.41
1:A:385:PHE:CE2	1:A:389:LEU:HD11	2.55	0.41
1:A:623:MET:HE3	1:A:698:TYR:CE2	2.56	0.41
1:A:885:THR:O	1:A:886:SER:HB2	2.20	0.41
1:A:1158:SER:O	1:A:1161:ASP:N	2.53	0.41
1:B:91:GLY:O	1:B:95:LEU:HG	2.21	0.41
1:B:127:LEU:HB3	1:B:180:VAL:HG21	2.03	0.41
1:B:141:LYS:O	1:B:142:GLU:HG3	2.20	0.41
1:B:169:TRP:CZ3	1:B:177:LEU:HB3	2.56	0.41
1:B:335:VAL:HG13	1:B:414:THR:HG21	2.02	0.41
1:B:915:PHE:CE2	1:B:988:LEU:HD21	2.56	0.41
1:B:1042:LEU:CD2	1:B:1084:VAL:HG12	2.51	0.41
1:B:1171:TYR:CE1	1:B:1256:ILE:HG12	2.56	0.41
1:B:1259:TYR:CE1	1:B:1263:LEU:HD11	2.56	0.41
1:C:503:GLN:HG2	1:C:541:LEU:HD21	2.03	0.41
1:C:664:ASP:OD1	1:C:664:ASP:N	2.54	0.41
1:C:1009:ILE:HG13	1:C:1009:ILE:H	1.66	0.41
1:C:1136:VAL:CG1	1:C:1198:LEU:HD12	2.51	0.41
1:D:211:PRO:HD3	1:D:267:VAL:HG13	2.03	0.41
1:D:385:PHE:CE2	1:D:389:LEU:HD11	2.55	0.41
1:D:565:GLN:H	1:D:565:GLN:HG2	1.53	0.41
1:D:814:THR:OG1	1:D:879:VAL:HG21	2.20	0.41
1:D:1272:VAL:HG12	1:D:1273:ASN:N	2.36	0.41
1:A:273:LEU:HD21	1:B:549:LEU:CD1	2.51	0.41
1:A:473:ILE:HG13	1:A:473:ILE:H	1.61	0.41
1:B:69:TYR:O	1:B:73:ILE:HG13	2.21	0.41
1:B:817:PHE:HB3	1:B:882:TRP:CE3	2.56	0.41
1:C:24:LEU:C	1:C:26:ASP:H	2.30	0.41
1:C:637:GLU:HB3	1:C:640:LEU:HG	2.03	0.41
1:C:705:LEU:HB3	1:C:755:TYR:CE2	2.55	0.41
1:D:169:TRP:CZ3	1:D:177:LEU:HB3	2.56	0.41
1:A:69:TYR:O	1:A:73:ILE:HG13	2.21	0.40
1:A:273:LEU:HD21	1:B:549:LEU:HD13	2.03	0.40
1:A:329:LEU:HD12	1:A:329:LEU:C	2.45	0.40
1:B:90:ILE:HG21	1:B:125:LYS:O	2.20	0.40
1:B:447:ARG:O	1:B:456:ILE:HD11	2.20	0.40
1:B:486:TYR:O	1:B:490:LEU:HG	2.22	0.40
1:B:814:THR:OG1	1:B:879:VAL:HG21	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:SER:HB3	1:B:999:PHE:HB3	2.02	0.40
1:C:1005:TRP:CZ2	1:C:1009:ILE:HD11	2.55	0.40
1:D:980:LEU:HD23	1:D:981:LEU:N	2.36	0.40
1:A:152:ASN:HB2	1:A:154:GLU:HG2	2.03	0.40
1:A:836:GLU:HA	1:A:839:HIS:NE2	2.36	0.40
1:A:880:LEU:HD22	1:A:907:CYS:HA	2.01	0.40
1:A:982:ILE:HD11	1:A:1024:LEU:HG	2.03	0.40
1:B:672:HIS:CE1	1:B:861:PRO:CD	3.04	0.40
1:C:95:LEU:O	1:C:98:HIS:CE1	2.74	0.40
1:C:661:GLU:HA	1:C:662:PRO:HD2	1.92	0.40
1:C:817:PHE:HB3	1:C:882:TRP:CE3	2.56	0.40
1:D:152:ASN:HB2	1:D:154:GLU:HG2	2.03	0.40
1:D:302:SER:CB	1:D:357:ARG:HG2	2.45	0.40
1:D:996:SER:HB3	1:D:999:PHE:HB3	2.02	0.40
1:D:1154:LEU:CD1	1:D:1163:LEU:HD12	2.45	0.40
1:A:927:GLN:O	1:A:931:GLN:HG3	2.22	0.40
1:A:930:LEU:HB3	1:A:950:ARG:HB3	2.03	0.40
1:A:982:ILE:HG21	1:A:1023:SER:HB3	2.03	0.40
1:B:201:MET:O	1:B:202:PHE:C	2.65	0.40
1:C:91:GLY:O	1:C:95:LEU:HG	2.21	0.40
1:C:177:LEU:O	1:C:180:VAL:HB	2.21	0.40
1:C:201:MET:O	1:C:202:PHE:C	2.64	0.40
1:C:391:ASP:OD2	1:C:447:ARG:NH1	2.54	0.40
1:C:931:GLN:HG2	1:C:950:ARG:NH1	2.36	0.40
1:A:217:LEU:HD22	1:A:229:VAL:CG1	2.41	0.40
1:A:817:PHE:HB3	1:A:882:TRP:CE3	2.56	0.40
1:A:996:SER:HB3	1:A:999:PHE:HB3	2.02	0.40
1:B:76:VAL:HG11	1:B:90:ILE:HD11	2.04	0.40
1:B:95:LEU:HA	1:B:98:HIS:HE1	1.86	0.40
1:B:474:LEU:HD22	1:B:477:CYS:SG	2.62	0.40
1:C:36:GLN:HG3	1:C:85:VAL:HG11	2.04	0.40
1:C:169:TRP:N	1:C:169:TRP:HD1	2.12	0.40
1:C:627:PHE:CE2	1:C:631:LYS:HD2	2.56	0.40
1:C:713:ILE:CG2	1:C:772:SER:HB3	2.50	0.40
1:C:1005:TRP:CE2	1:C:1009:ILE:HD11	2.56	0.40
1:A:177:LEU:O	1:A:180:VAL:HB	2.21	0.40
1:A:277:PHE:HZ	1:B:551:SER:C	2.29	0.40
1:A:565:GLN:H	1:A:565:GLN:HG2	1.53	0.40
1:A:664:ASP:OD1	1:A:664:ASP:N	2.54	0.40
1:A:1259:TYR:CE1	1:A:1263:LEU:HD11	2.56	0.40
1:B:95:LEU:O	1:B:98:HIS:CE1	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:SER:O	1:B:767:PHE:CD1	2.72	0.40
1:B:913:LYS:O	1:B:917:VAL:HG23	2.21	0.40
1:C:814:THR:OG1	1:C:879:VAL:HG21	2.20	0.40
1:C:815:ALA:HA	1:C:819:ASP:HB3	2.04	0.40
1:C:1042:LEU:O	1:C:1145:PHE:HD1	2.04	0.40
1:D:549:LEU:HB2	1:D:567:ARG:CD	2.52	0.40
1:D:836:GLU:HA	1:D:839:HIS:NE2	2.36	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	1108/1308 (85%)	1023 (92%)	82 (7%)	3 (0%)	36	65
1	B	1045/1308 (80%)	969 (93%)	72 (7%)	4 (0%)	30	60
1	C	1108/1308 (85%)	1022 (92%)	83 (8%)	3 (0%)	36	65
1	D	1008/1308 (77%)	933 (93%)	71 (7%)	4 (0%)	30	60
All	All	4269/5232 (82%)	3947 (92%)	308 (7%)	14 (0%)	36	65

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	150	ASP
1	B	122	VAL
1	B	150	ASP
1	C	122	VAL
1	C	150	ASP
1	D	122	VAL
1	D	150	ASP

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Mol	Chain	Res	Type
1	A	996	SER
1	B	996	SER
1	C	996	SER
1	D	452	THR
1	D	996	SER
1	B	452	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1032/1188 (87%)	902 (87%)	130 (13%)	4	18
1	B	979/1188 (82%)	852 (87%)	127 (13%)	4	17
1	C	1032/1188 (87%)	898 (87%)	134 (13%)	4	17
1	D	945/1188 (80%)	823 (87%)	122 (13%)	4	17
All	All	3988/4752 (84%)	3475 (87%)	513 (13%)	4	17

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	19	GLU
1	A	29	LEU
1	A	36	GLN
1	A	43	VAL
1	A	54	SER
1	A	71	CYS
1	A	81	LEU
1	A	96	GLU
1	A	97	VAL
1	A	99	HIS
1	A	118	GLU
1	A	119	ASP
1	A	130	LEU
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	169	TRP
1	A	177	LEU
1	A	183	ASP
1	A	200	THR
1	A	208	GLN
1	A	213	LEU
1	A	240	LEU
1	A	247	GLU
1	A	262	ASP
1	A	264	LEU
1	A	273	LEU
1	A	275	ILE
1	A	285	LEU
1	A	288	GLU
1	A	312	LEU
1	A	316	LEU
1	A	320	GLN
1	A	329	LEU
1	A	343	LEU
1	A	347	SER
1	A	349	PHE
1	A	360	VAL
1	A	376	ASP
1	A	377	HIS
1	A	378	VAL
1	A	383	ILE
1	A	396	LYS
1	A	398	ILE
1	A	413	MET
1	A	414	THR
1	A	421	LEU
1	A	427	LEU
1	A	438	GLN
1	A	443	GLN
1	A	450	THR
1	A	451	ARG
1	A	452	THR
1	A	456	ILE
1	A	468	MET
1	A	473	ILE
1	A	477	CYS
1	A	479	LYS

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Mol	Chain	Res	Type
1	A	483	THR
1	A	488	THR
1	A	493	GLN
1	A	496	GLN
1	A	502	VAL
1	A	515	SER
1	A	517	ILE
1	A	519	VAL
1	A	529	LEU
1	A	530	ASP
1	A	548	VAL
1	A	549	LEU
1	A	552	LEU
1	A	563	VAL
1	A	565	GLN
1	A	569	ASP
1	A	579	ASN
1	A	587	ILE
1	A	597	GLN
1	A	600	ILE
1	A	612	LEU
1	A	639	ASP
1	A	651	LEU
1	A	659	LEU
1	A	663	LEU
1	A	666	LEU
1	A	699	SER
1	A	711	ARG
1	A	712	MET
1	A	743	CYS
1	A	754	GLU
1	A	759	ILE
1	A	765	SER
1	A	766	LYS
1	A	768	GLU
1	A	771	LEU
1	A	801	ASP
1	A	803	LEU
1	A	806	LEU
1	A	812	LEU
1	A	824	HIS
1	A	838	MET

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Mol	Chain	Res	Type
1	A	846	LEU
1	A	853	ILE
1	A	858	VAL
1	A	864	GLN
1	A	911	LEU
1	A	919	LEU
1	A	949	GLN
1	A	954	GLN
1	A	965	LEU
1	A	980	LEU
1	A	981	LEU
1	A	982	ILE
1	A	1001	GLN
1	A	1003	LEU
1	A	1013	TYR
1	A	1015	GLN
1	A	1024	LEU
1	A	1049	ILE
1	A	1050	HIS
1	A	1056	ILE
1	A	1071	VAL
1	A	1084	VAL
1	A	1105	SER
1	A	1142	LEU
1	A	1154	LEU
1	A	1183	GLN
1	A	1184	VAL
1	A	1194	THR
1	A	1249	ILE
1	A	1274	LEU
1	A	1275	MET
1	B	71	CYS
1	B	81	LEU
1	B	96	GLU
1	B	97	VAL
1	B	99	HIS
1	B	118	GLU
1	B	119	ASP
1	B	130	LEU
1	B	164	LEU
1	B	169	TRP
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	183	ASP
1	B	200	THR
1	B	208	GLN
1	B	213	LEU
1	B	240	LEU
1	B	247	GLU
1	B	262	ASP
1	B	264	LEU
1	B	273	LEU
1	B	275	ILE
1	B	277	PHE
1	B	285	LEU
1	B	288	GLU
1	B	297	GLN
1	B	312	LEU
1	B	316	LEU
1	B	320	GLN
1	B	329	LEU
1	B	343	LEU
1	B	347	SER
1	B	349	PHE
1	B	360	VAL
1	B	376	ASP
1	B	377	HIS
1	B	378	VAL
1	B	383	ILE
1	B	396	LYS
1	B	398	ILE
1	B	413	MET
1	B	414	THR
1	B	421	LEU
1	B	427	LEU
1	B	438	GLN
1	B	443	GLN
1	B	450	THR
1	B	451	ARG
1	B	452	THR
1	B	456	ILE
1	B	473	ILE
1	B	477	CYS
1	B	479	LYS
1	B	483	THR

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Mol	Chain	Res	Type
1	B	488	THR
1	B	493	GLN
1	B	496	GLN
1	B	498	LEU
1	B	502	VAL
1	B	515	SER
1	B	517	ILE
1	B	519	VAL
1	B	529	LEU
1	B	530	ASP
1	B	548	VAL
1	B	549	LEU
1	B	552	LEU
1	B	563	VAL
1	B	565	GLN
1	B	569	ASP
1	B	579	ASN
1	B	587	ILE
1	B	597	GLN
1	B	600	ILE
1	B	612	LEU
1	B	639	ASP
1	B	651	LEU
1	B	659	LEU
1	B	663	LEU
1	B	666	LEU
1	B	699	SER
1	B	711	ARG
1	B	712	MET
1	B	743	CYS
1	B	754	GLU
1	B	759	ILE
1	B	765	SER
1	B	766	LYS
1	B	768	GLU
1	B	771	LEU
1	B	801	ASP
1	B	803	LEU
1	B	806	LEU
1	B	812	LEU
1	B	824	HIS
1	B	838	MET

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Mol	Chain	Res	Type
1	B	846	LEU
1	B	853	ILE
1	B	858	VAL
1	B	864	GLN
1	B	911	LEU
1	B	919	LEU
1	B	949	GLN
1	B	954	GLN
1	B	965	LEU
1	B	980	LEU
1	B	981	LEU
1	B	982	ILE
1	B	1001	GLN
1	B	1003	LEU
1	B	1009	ILE
1	B	1013	TYR
1	B	1015	GLN
1	B	1024	LEU
1	B	1049	ILE
1	B	1050	HIS
1	B	1056	ILE
1	B	1071	VAL
1	B	1084	VAL
1	B	1105	SER
1	B	1142	LEU
1	B	1154	LEU
1	B	1183	GLN
1	B	1184	VAL
1	B	1194	THR
1	B	1249	ILE
1	B	1274	LEU
1	B	1275	MET
1	C	15	ASP
1	C	19	GLU
1	C	29	LEU
1	C	36	GLN
1	C	43	VAL
1	C	54	SER
1	C	71	CYS
1	C	81	LEU
1	C	96	GLU
1	C	97	VAL

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Mol	Chain	Res	Type
1	C	99	HIS
1	C	118	GLU
1	C	119	ASP
1	C	130	LEU
1	C	164	LEU
1	C	169	TRP
1	C	177	LEU
1	C	183	ASP
1	C	200	THR
1	C	203	SER
1	C	208	GLN
1	C	213	LEU
1	C	240	LEU
1	C	247	GLU
1	C	262	ASP
1	C	264	LEU
1	C	273	LEU
1	C	275	ILE
1	C	277	PHE
1	C	285	LEU
1	C	288	GLU
1	C	297	GLN
1	C	312	LEU
1	C	316	LEU
1	C	329	LEU
1	C	343	LEU
1	C	347	SER
1	C	349	PHE
1	C	352	THR
1	C	360	VAL
1	C	376	ASP
1	C	377	HIS
1	C	378	VAL
1	C	383	ILE
1	C	396	LYS
1	C	398	ILE
1	C	413	MET
1	C	414	THR
1	C	421	LEU
1	C	427	LEU
1	C	438	GLN
1	C	443	GLN

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Mol	Chain	Res	Type
1	C	450	THR
1	C	451	ARG
1	C	452	THR
1	C	456	ILE
1	C	468	MET
1	C	473	ILE
1	C	477	CYS
1	C	479	LYS
1	C	483	THR
1	C	488	THR
1	C	493	GLN
1	C	496	GLN
1	C	502	VAL
1	C	515	SER
1	C	517	ILE
1	C	519	VAL
1	C	529	LEU
1	C	530	ASP
1	C	548	VAL
1	C	549	LEU
1	C	552	LEU
1	C	563	VAL
1	C	565	GLN
1	C	569	ASP
1	C	579	ASN
1	C	587	ILE
1	C	597	GLN
1	C	600	ILE
1	C	612	LEU
1	C	639	ASP
1	C	651	LEU
1	C	659	LEU
1	C	663	LEU
1	C	666	LEU
1	C	699	SER
1	C	711	ARG
1	C	712	MET
1	C	743	CYS
1	C	754	GLU
1	C	759	ILE
1	C	765	SER
1	C	766	LYS

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Mol	Chain	Res	Type
1	C	768	GLU
1	C	771	LEU
1	C	801	ASP
1	C	803	LEU
1	C	806	LEU
1	C	812	LEU
1	C	824	HIS
1	C	838	MET
1	C	846	LEU
1	C	853	ILE
1	C	858	VAL
1	C	864	GLN
1	C	911	LEU
1	C	919	LEU
1	C	949	GLN
1	C	954	GLN
1	C	965	LEU
1	C	980	LEU
1	C	981	LEU
1	C	982	ILE
1	C	1001	GLN
1	C	1003	LEU
1	C	1009	ILE
1	C	1013	TYR
1	C	1015	GLN
1	C	1024	LEU
1	C	1049	ILE
1	C	1050	HIS
1	C	1056	ILE
1	C	1071	VAL
1	C	1084	VAL
1	C	1105	SER
1	C	1142	LEU
1	C	1154	LEU
1	C	1183	GLN
1	C	1184	VAL
1	C	1194	THR
1	C	1249	ILE
1	C	1274	LEU
1	C	1275	MET
1	D	118	GLU
1	D	119	ASP

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Mol	Chain	Res	Type
1	D	130	LEU
1	D	164	LEU
1	D	169	TRP
1	D	177	LEU
1	D	183	ASP
1	D	200	THR
1	D	208	GLN
1	D	213	LEU
1	D	240	LEU
1	D	247	GLU
1	D	262	ASP
1	D	264	LEU
1	D	273	LEU
1	D	275	ILE
1	D	277	PHE
1	D	285	LEU
1	D	288	GLU
1	D	297	GLN
1	D	312	LEU
1	D	316	LEU
1	D	329	LEU
1	D	343	LEU
1	D	347	SER
1	D	349	PHE
1	D	360	VAL
1	D	376	ASP
1	D	377	HIS
1	D	378	VAL
1	D	383	ILE
1	D	396	LYS
1	D	398	ILE
1	D	413	MET
1	D	414	THR
1	D	421	LEU
1	D	427	LEU
1	D	438	GLN
1	D	443	GLN
1	D	450	THR
1	D	451	ARG
1	D	452	THR
1	D	456	ILE
1	D	468	MET

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Mol	Chain	Res	Type
1	D	473	ILE
1	D	477	CYS
1	D	479	LYS
1	D	483	THR
1	D	488	THR
1	D	493	GLN
1	D	496	GLN
1	D	498	LEU
1	D	502	VAL
1	D	515	SER
1	D	517	ILE
1	D	519	VAL
1	D	529	LEU
1	D	530	ASP
1	D	548	VAL
1	D	549	LEU
1	D	552	LEU
1	D	563	VAL
1	D	565	GLN
1	D	569	ASP
1	D	579	ASN
1	D	587	ILE
1	D	597	GLN
1	D	600	ILE
1	D	612	LEU
1	D	639	ASP
1	D	651	LEU
1	D	659	LEU
1	D	663	LEU
1	D	666	LEU
1	D	699	SER
1	D	711	ARG
1	D	712	MET
1	D	743	CYS
1	D	754	GLU
1	D	759	ILE
1	D	765	SER
1	D	766	LYS
1	D	768	GLU
1	D	771	LEU
1	D	801	ASP
1	D	803	LEU

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Mol	Chain	Res	Type
1	D	806	LEU
1	D	812	LEU
1	D	824	HIS
1	D	838	MET
1	D	846	LEU
1	D	853	ILE
1	D	858	VAL
1	D	864	GLN
1	D	911	LEU
1	D	919	LEU
1	D	949	GLN
1	D	954	GLN
1	D	965	LEU
1	D	980	LEU
1	D	981	LEU
1	D	982	ILE
1	D	1001	GLN
1	D	1003	LEU
1	D	1009	ILE
1	D	1013	TYR
1	D	1015	GLN
1	D	1024	LEU
1	D	1049	ILE
1	D	1050	HIS
1	D	1056	ILE
1	D	1071	VAL
1	D	1084	VAL
1	D	1105	SER
1	D	1142	LEU
1	D	1154	LEU
1	D	1183	GLN
1	D	1184	VAL
1	D	1194	THR
1	D	1249	ILE
1	D	1274	LEU
1	D	1275	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	298	GLN

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Mol	Chain	Res	Type
1	A	320	GLN
1	A	351	GLN
1	A	377	HIS
1	A	438	GLN
1	A	565	GLN
1	A	597	GLN
1	A	672	HIS
1	A	756	ASN
1	A	761	ASN
1	A	847	GLN
1	A	959	GLN
1	A	1015	GLN
1	A	1218	GLN
1	A	1251	ASN
1	B	216	GLN
1	B	320	GLN
1	B	351	GLN
1	B	377	HIS
1	B	433	HIS
1	B	458	HIS
1	B	565	GLN
1	B	597	GLN
1	B	665	HIS
1	B	672	HIS
1	B	761	ASN
1	B	847	GLN
1	B	1251	ASN
1	C	216	GLN
1	C	377	HIS
1	C	565	GLN
1	C	672	HIS
1	C	756	ASN
1	C	761	ASN
1	C	847	GLN
1	C	959	GLN
1	C	1251	ASN
1	D	216	GLN
1	D	351	GLN
1	D	377	HIS
1	D	433	HIS
1	D	458	HIS
1	D	565	GLN

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Mol	Chain	Res	Type
1	D	665	HIS
1	D	672	HIS
1	D	761	ASN
1	D	847	GLN
1	D	959	GLN
1	D	1251	ASN

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1134/1308 (86%)	0.31	68 (5%)	27	19	85, 192, 306, 410	0
1	B	1071/1308 (81%)	0.08	17 (1%)	70	52	87, 188, 306, 415	0
1	C	1134/1308 (86%)	0.33	61 (5%)	31	21	81, 191, 306, 410	0
1	D	1034/1308 (79%)	0.13	25 (2%)	59	40	84, 185, 302, 416	0
All	All	4373/5232 (83%)	0.21	171 (3%)	43	29	81, 189, 304, 416	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	ILE	5.5
1	A	845	THR	5.4
1	A	1214	ILE	5.4
1	C	110	SER	5.4
1	A	160	LEU	5.0
1	C	105	LEU	4.7
1	C	112	PHE	4.6
1	C	109	ALA	4.6
1	A	127	LEU	4.3
1	A	156	TYR	4.3
1	D	109	ALA	4.2
1	C	134	LEU	4.1
1	C	113	VAL	4.0
1	C	73	ILE	4.0
1	C	170	PRO	3.9
1	A	113	VAL	3.9
1	A	72	CYS	3.9
1	A	106	VAL	3.9
1	C	116	VAL	3.8
1	C	28	ASP	3.8
1	A	1210	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	135	THR	3.8
1	A	116	VAL	3.7
1	C	106	VAL	3.6
1	C	130	LEU	3.6
1	B	181	PHE	3.6
1	D	1049	ILE	3.6
1	A	110	SER	3.5
1	C	102	GLY	3.5
1	C	127	LEU	3.5
1	A	102	GLY	3.5
1	C	181	PHE	3.5
1	D	116	VAL	3.5
1	A	109	ALA	3.5
1	A	134	LEU	3.4
1	C	161	ILE	3.4
1	D	301	PRO	3.4
1	A	130	LEU	3.3
1	C	77	GLU	3.3
1	C	121	LEU	3.3
1	D	181	PHE	3.3
1	C	72	CYS	3.3
1	D	1274	LEU	3.3
1	A	169	TRP	3.3
1	C	178	THR	3.2
1	A	164	LEU	3.2
1	D	126	SER	3.2
1	A	112	PHE	3.1
1	A	105	LEU	3.1
1	C	145	ALA	3.1
1	C	177	LEU	3.1
1	C	1210	CYS	3.1
1	A	133	ILE	3.1
1	A	1042	LEU	3.1
1	B	178	THR	3.1
1	C	97	VAL	3.1
1	A	103	PRO	3.1
1	A	963	LEU	3.0
1	C	122	VAL	3.0
1	C	175	ILE	3.0
1	A	161	ILE	3.0
1	C	123	ASN	3.0
1	C	137	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	169	TRP	2.9
1	A	177	LEU	2.9
1	A	153	GLY	2.9
1	A	849	ILE	2.8
1	C	165	CYS	2.8
1	A	73	ILE	2.8
1	B	1146	PHE	2.8
1	A	1217	VAL	2.8
1	A	69	TYR	2.8
1	D	799	VAL	2.8
1	B	126	SER	2.8
1	D	130	LEU	2.8
1	A	165	CYS	2.7
1	A	411	SER	2.7
1	C	126	SER	2.7
1	A	97	VAL	2.7
1	C	108	LEU	2.7
1	C	164	LEU	2.7
1	D	134	LEU	2.7
1	B	89	ILE	2.7
1	A	146	CYS	2.7
1	C	167	VAL	2.6
1	C	173	TYR	2.6
1	A	1049	ILE	2.6
1	A	181	PHE	2.6
1	C	101	PRO	2.6
1	C	1072	ASN	2.6
1	D	112	PHE	2.6
1	A	129	LEU	2.6
1	C	119	ASP	2.6
1	A	1045	LEU	2.6
1	B	134	LEU	2.6
1	D	553	PRO	2.5
1	C	89	ILE	2.5
1	A	1159	CYS	2.5
1	D	113	VAL	2.5
1	A	124	GLY	2.5
1	A	841	ALA	2.5
1	B	553	PRO	2.5
1	C	698	TYR	2.5
1	B	109	ALA	2.5
1	A	977	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	175	ILE	2.5
1	A	131	PRO	2.5
1	A	170	PRO	2.5
1	C	712	MET	2.4
1	A	101	PRO	2.4
1	A	66	TYR	2.4
1	B	411	SER	2.4
1	A	776	CYS	2.4
1	C	930	LEU	2.4
1	A	178	THR	2.4
1	C	103	PRO	2.4
1	C	1071	VAL	2.4
1	D	475	GLN	2.4
1	A	63	LEU	2.4
1	C	933	LEU	2.4
1	B	1191	ILE	2.3
1	D	299	GLY	2.3
1	C	160	LEU	2.3
1	C	69	TYR	2.3
1	A	123	ASN	2.3
1	A	151	LEU	2.3
1	A	799	VAL	2.3
1	A	174	MET	2.3
1	C	641	LEU	2.3
1	D	1217	VAL	2.3
1	B	301	PRO	2.3
1	C	301	PRO	2.3
1	C	131	PRO	2.2
1	A	144	LEU	2.2
1	C	411	SER	2.2
1	A	43	VAL	2.2
1	C	146	CYS	2.2
1	A	884	TYR	2.2
1	C	66	TYR	2.2
1	D	260	PRO	2.2
1	D	155	GLU	2.2
1	C	608	PHE	2.2
1	A	167	VAL	2.2
1	A	126	SER	2.2
1	D	411	SER	2.2
1	D	1056	ILE	2.2
1	A	215	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	849	ILE	2.1
1	C	129	LEU	2.1
1	C	1149	LEU	2.1
1	A	29	LEU	2.1
1	A	121	LEU	2.1
1	B	148	LYS	2.1
1	A	967	SER	2.1
1	B	116	VAL	2.1
1	B	570	VAL	2.1
1	A	163	THR	2.1
1	C	75	LEU	2.1
1	A	104	LEU	2.1
1	B	260	PRO	2.1
1	A	47	LEU	2.1
1	D	1191	ILE	2.1
1	A	1198	LEU	2.0
1	D	552	LEU	2.0
1	D	165	CYS	2.0
1	C	298	GLN	2.0
1	A	117	ARG	2.0
1	B	800	SER	2.0
1	C	400	ASP	2.0
1	B	1145	PHE	2.0
1	A	188	PRO	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 oligosaccharides 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.