Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:18 AM GMT

PDB ID	:	2WLN
Title	:	POTASSIUM CHANNEL FROM MAGNETOSPIRILLUM MAGNETOTACTICUM
Authors	:	Clarke, O.B.; Caputo, A.T.; Smith, B.J.; Gulbis, J.M.
Deposited on	:	2009-06-24
Resolution	:	3.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

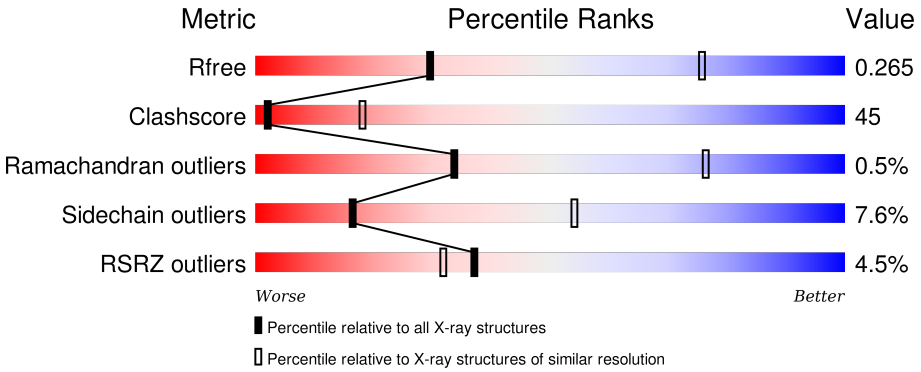
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.44 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}	91344	1007 (3.54-3.34)
Clashscore	102246	1044 (3.52-3.36)
Ramachandran outliers	100387	1013 (3.52-3.36)
Sidechain outliers	100360	1014 (3.52-3.36)
RSRZ outliers	91569	1012 (3.54-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	301	5% 39% 50% 5% 6%
1	B	301	3% 43% 46% 5% 6%
1	C	301	3% 41% 47% 6% 6%
1	D	301	4% 45% 43% 6% 6%
1	E	301	5% 41% 47% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	301	4% 43% 45% 6% 6%
1	G	301	5% 42% 47% 5% 6%
1	H	301	4% 44% 44% 7% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17667 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 POTASSIUM CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2206	1417	383	398	8			
1	B	283	Total	C	N	O	S	0	0	0
			2205	1418	380	398	9			
1	C	283	Total	C	N	O	S	0	0	0
			2205	1418	380	398	9			
1	D	283	Total	C	N	O	S	0	0	0
			2214	1426	381	398	9			
1	E	283	Total	C	N	O	S	0	0	0
			2209	1421	381	398	9			
1	F	283	Total	C	N	O	S	0	0	0
			2209	1419	383	398	9			
1	G	283	Total	C	N	O	S	0	0	0
			2205	1418	380	398	9			
1	H	283	Total	C	N	O	S	0	0	0
			2208	1419	382	398	9			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

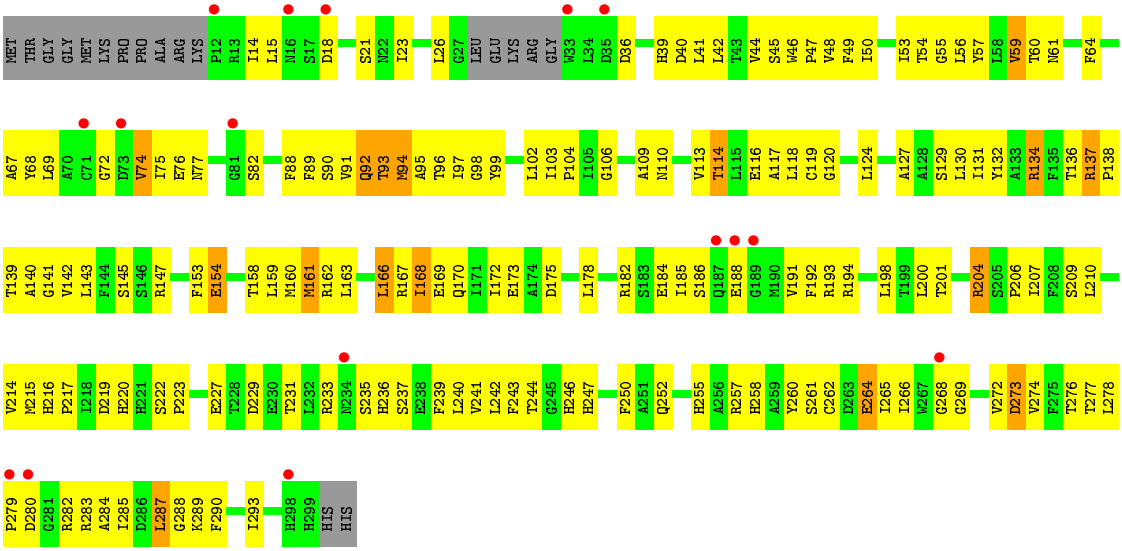
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	K	0	0
			1	1		
2	A	2	Total	K	0	0
			2	2		
2	C	1	Total	K	0	0
			1	1		
2	F	2	Total	K	0	0
			2	2		

3 Residue-property plots (i)

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

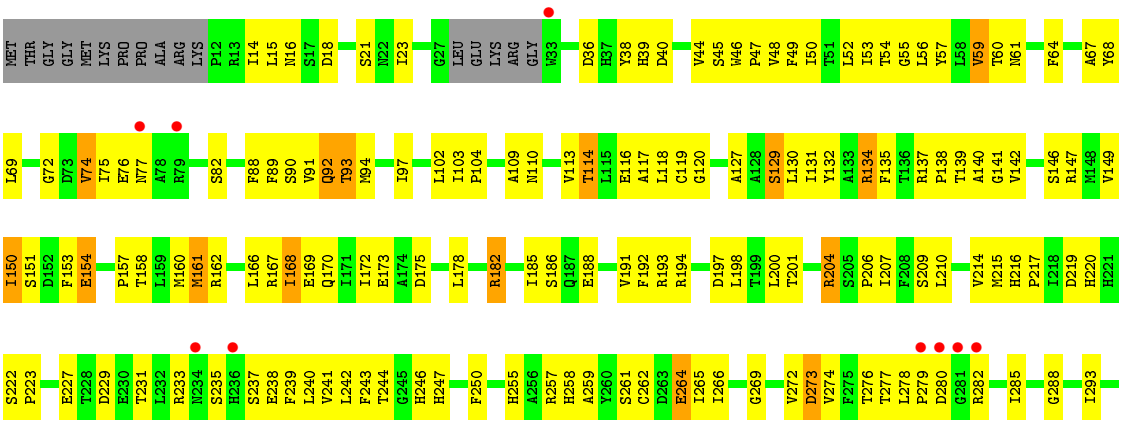
- Molecule 1: POTASSIUM CHANNEL

Chain A:



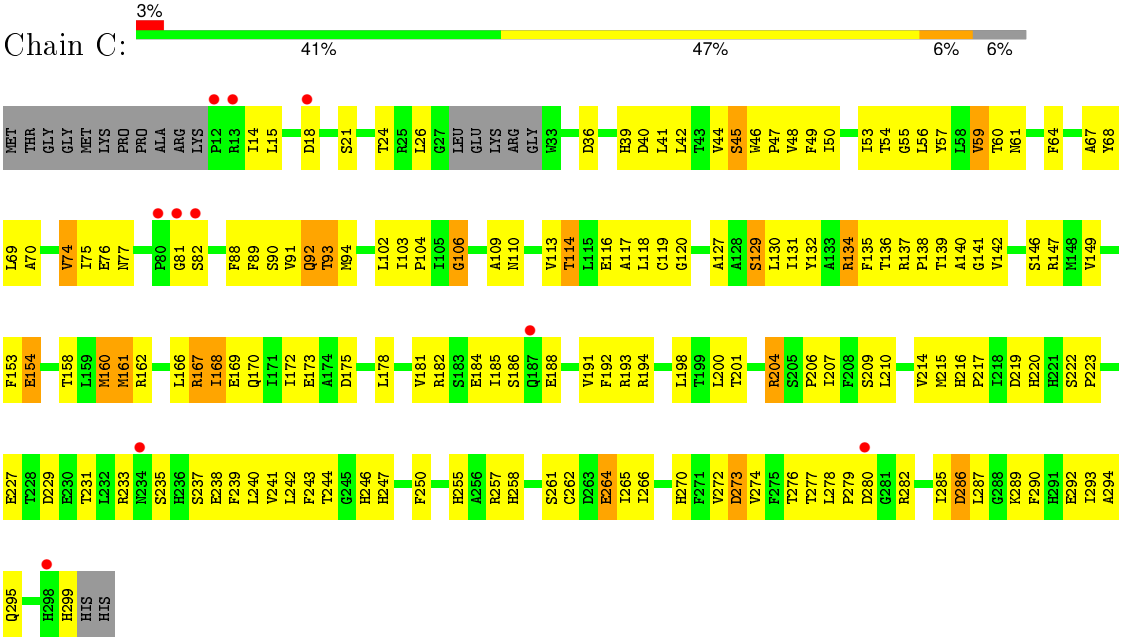
- Molecule 1: POTASSIUM CHANNEL

Chain B:



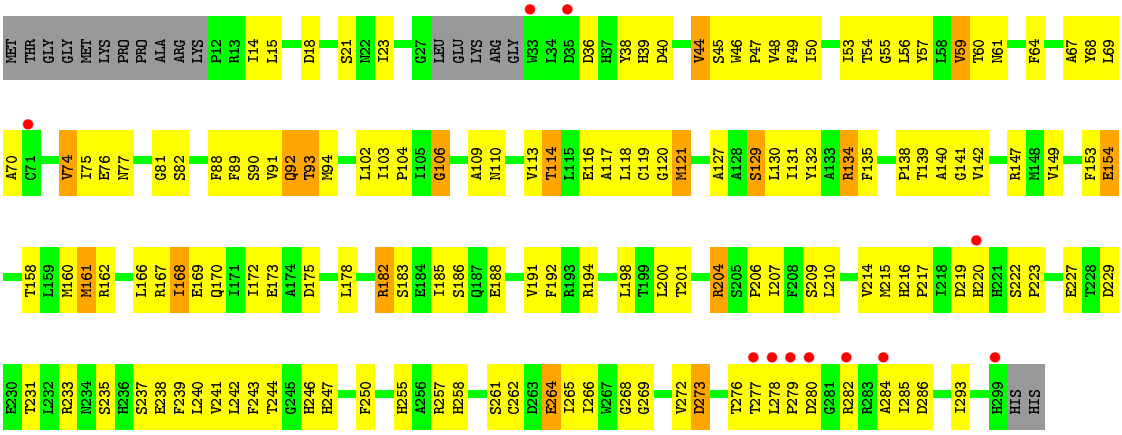
• Molecule 1: POTASSIUM CHANNEL

Chain C:



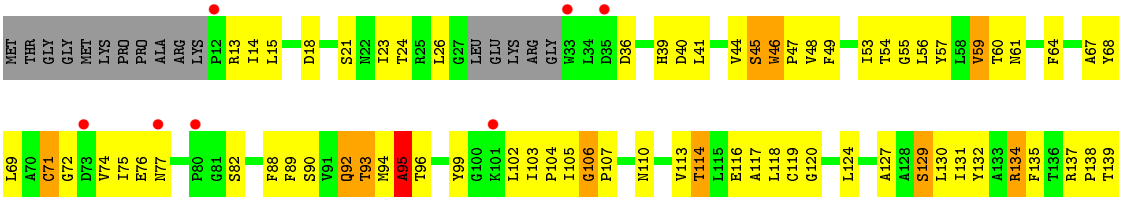
• Molecule 1: POTASSIUM CHANNEL

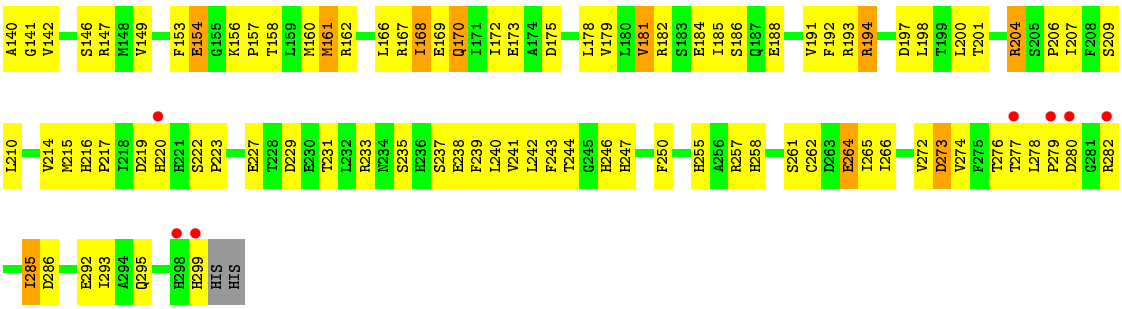
Chain D:



• Molecule 1: POTASSIUM CHANNEL

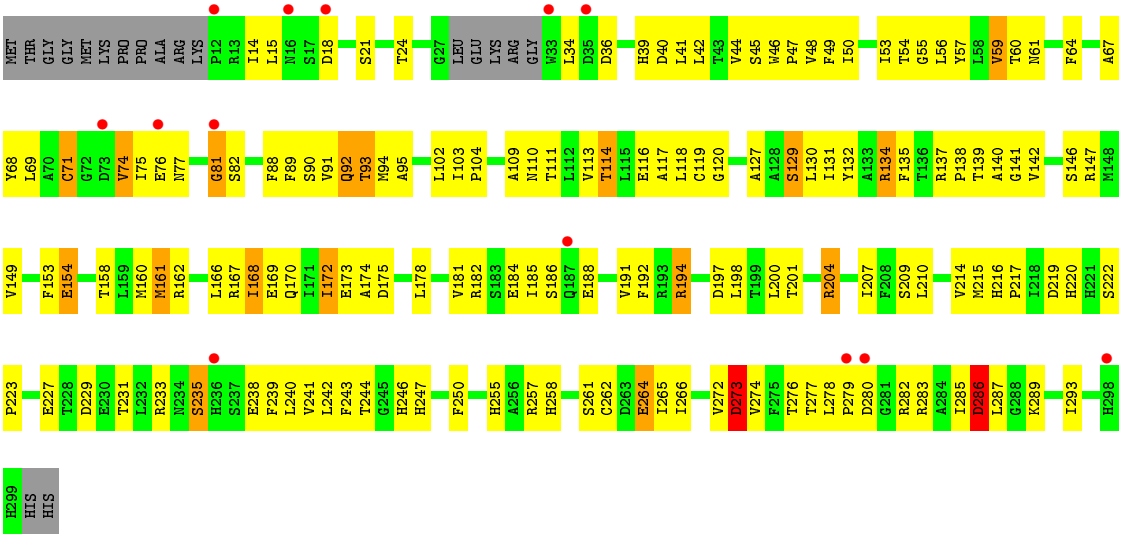
Chain E:





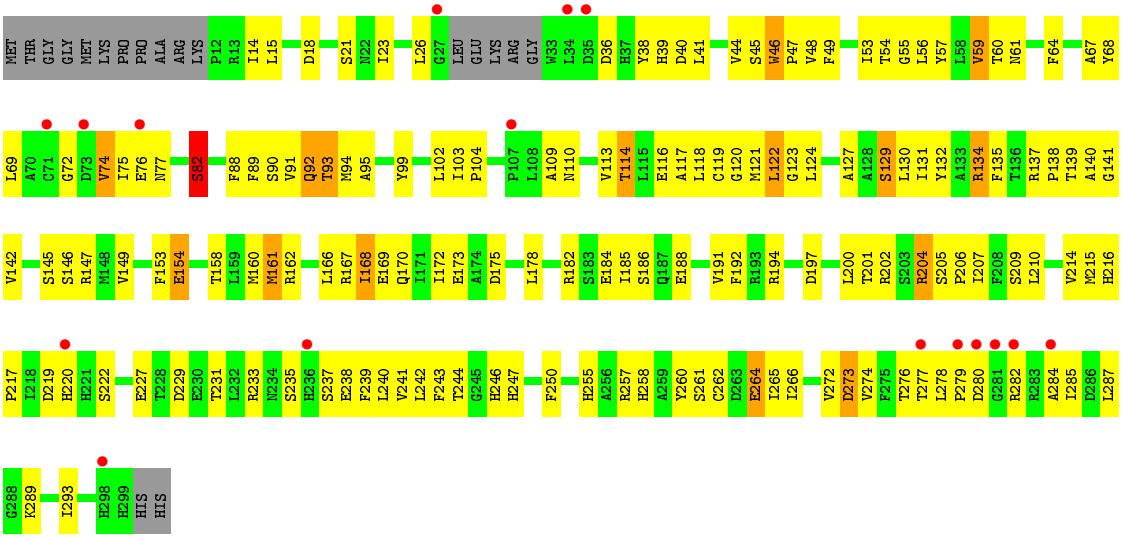
• Molecule 1: POTASSIUM CHANNEL

Chain F:



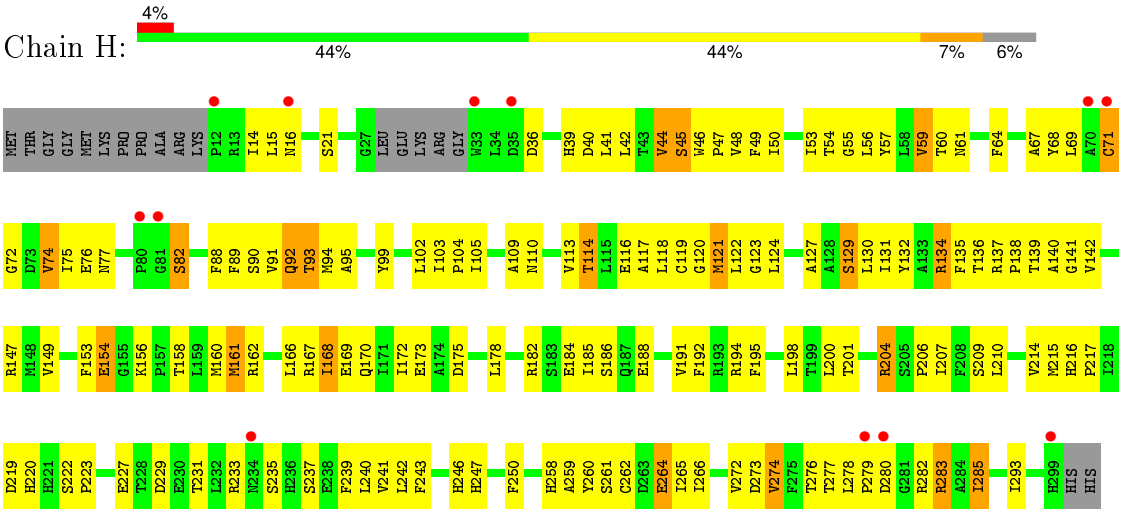
• Molecule 1: POTASSIUM CHANNEL

Chain G:



• Molecule 1: POTASSIUM CHANNEL

Chain H:


4%
44%
44%
7%
6%
MET THR GLY GLY MET LYS PRO PRO ALA ARG LYS P12 R13 I14 L15 N16 S21 G27 LEU GLU LYS ARG GLY W33 L34 D35 D36 H39 D40 L41 L42 T43 V44 S45 W46 P47 V48 F49 I50 I53 T54 G55 L56 Y57 L58 V59 T60 N61 F64 A67 Y68 L69 A70 G71
G72 D73 V74 I75 E76 N77 P80 G81 S82 F88 F89 S90 V91 Q92 T93 M94 A95 Y99 L102 I103 P104 I105 A109 N110 V113 T114 L115 E116 A117 L118 C119 G120 M121 L122 G123 L124 A127 A128 S129 L130 I131 Y132 A133 R134 F135 T136 R137 P138 T139 A140 G141 V142
R147 M148 V149 F153 E154 G155 K156 P157 T158 L159 M160 M161 R162 L166 R167 I168 E169 Q170 I171 I172 E173 A174 D175 L178 R182 S183 E184 I185 S186 Q187 E188 V191 F192 R193 R194 F195 L198 T199 L200 T201 R204 S205 P206 I207 F208 S209 L210 V214 M215 H216 P217 I218
D219 H220 H221 S222 P223 E227 T228 D229 E230 T231 I232 R233 M234 S235 H236 S237 E238 F239 L240 V241 I242 F243 H246 H247 F250 H258 A259 Y260 S261 C262 D263 E264 I265 I266 V272 D273 V274 F275 T276 T277 L278 P279 D280 G281 R282 R283 A284 I285 I293 H299 HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	106.68Å 109.06Å 146.39Å 73.95° 82.30° 89.88°	Depositor
Resolution (Å)	15.00 – 3.44 15.00 – 3.44	Depositor EDS
% Data completeness (in resolution range)	93.2 (15.00-3.44) 68.3 (15.00-3.44)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.266 , 0.273 0.254 , 0.265	Depositor DCC
R_{free} test set	3196 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	93.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 62319 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17667	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	1.13	8/2263 (0.4%)	0.78	6/3082 (0.2%)
1	B	0.87	7/2262 (0.3%)	0.71	1/3080 (0.0%)
1	C	0.75	4/2262 (0.2%)	0.81	9/3080 (0.3%)
1	D	0.85	6/2273 (0.3%)	0.88	8/3096 (0.3%)
1	E	1.04	10/2266 (0.4%)	0.84	11/3084 (0.4%)
1	F	0.78	6/2266 (0.3%)	1.00	13/3085 (0.4%)
1	G	0.95	7/2262 (0.3%)	0.69	0/3080
1	H	0.89	7/2264 (0.3%)	0.86	11/3081 (0.4%)
All	All	0.92	55/18118 (0.3%)	0.83	59/24668 (0.2%)

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	B	0	1
1	C	0	1
1	E	0	1
1	F	0	4
1	G	0	1
All	All	0	8

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	LEU	C-N	-32.15	0.75	1.33
1	E	71	CYS	C-N	20.88	1.70	1.33
1	G	122	LEU	C-N	-20.53	0.96	1.33
1	A	94	MET	C-N	-20.27	0.87	1.34
1	G	287	LEU	C-N	-20.22	0.96	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	82	SER	C-N	-20.21	0.87	1.34
1	E	106	GLY	C-N	19.34	1.71	1.34
1	B	157	PRO	C-N	-17.95	0.92	1.34
1	D	182	ARG	C-N	15.61	1.70	1.34
1	H	274	VAL	C-N	-14.08	1.01	1.34
1	F	172	ILE	C-N	-13.69	1.02	1.34
1	B	150	ILE	C-N	13.65	1.65	1.34
1	E	95	ALA	C-N	-13.36	1.03	1.34
1	E	285	ILE	C-N	-12.72	1.04	1.34
1	B	273	ASP	C-N	12.62	1.63	1.34
1	D	273	ASP	C-N	12.50	1.62	1.34
1	C	70	ALA	C-N	12.43	1.62	1.34
1	A	268	GLY	C-N	11.73	1.54	1.33
1	E	137	ARG	C-N	10.75	1.54	1.34
1	F	81	GLY	C-N	-9.82	1.11	1.34
1	A	106	GLY	C-N	-9.70	1.15	1.34
1	A	159	LEU	C-N	9.66	1.56	1.34
1	D	268	GLY	C-N	9.61	1.50	1.33
1	D	106	GLY	C-N	-9.47	1.16	1.34
1	G	95	ALA	C-N	9.35	1.55	1.34
1	G	46	TRP	C-N	-9.25	1.16	1.34
1	D	70	ALA	C-N	9.10	1.54	1.34
1	A	166	LEU	C-N	8.83	1.54	1.34
1	B	288	GLY	C-N	-8.68	1.14	1.34
1	H	260	TYR	C-N	8.65	1.53	1.34
1	H	195	PHE	C-N	-8.34	1.14	1.34
1	A	273	ASP	C-N	-7.72	1.16	1.34
1	D	286	ASP	C-N	-7.68	1.16	1.34
1	G	137	ARG	C-N	7.52	1.48	1.34
1	G	82	SER	C-N	-7.48	1.16	1.34
1	C	81	GLY	C-N	-7.45	1.17	1.34
1	F	71	CYS	C-N	7.19	1.46	1.33
1	E	286	ASP	C-N	-7.02	1.17	1.34
1	E	273	ASP	C-N	6.97	1.50	1.34
1	A	137	ARG	C-N	6.74	1.47	1.34
1	F	181	VAL	C-N	6.68	1.49	1.34
1	E	181	VAL	C-N	6.61	1.49	1.34
1	C	160	MET	C-N	6.57	1.49	1.34
1	H	44	VAL	C-N	6.03	1.48	1.34
1	C	106	GLY	C-N	6.01	1.45	1.34
1	G	273	ASP	C-N	-5.85	1.20	1.34
1	F	95	ALA	C-N	5.72	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	274	VAL	C-N	5.71	1.47	1.34
1	H	45	SER	C-N	5.48	1.46	1.34
1	F	194	ARG	C-N	-5.32	1.21	1.34
1	B	182	ARG	C-N	5.21	1.46	1.34
1	H	95	ALA	C-N	-5.20	1.22	1.34
1	B	193	ARG	C-N	-5.12	1.22	1.34
1	B	137	ARG	C-N	5.10	1.44	1.34
1	E	46	TRP	C-N	-5.06	1.24	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	286	ASP	O-C-N	-20.18	90.41	122.70
1	D	286	ASP	O-C-N	-16.18	96.81	122.70
1	F	81	GLY	O-C-N	-14.45	99.59	122.70
1	D	81	GLY	O-C-N	-13.70	100.78	122.70
1	F	273	ASP	O-C-N	-13.56	101.00	122.70
1	C	286	ASP	O-C-N	-13.25	101.50	122.70
1	F	286	ASP	CA-C-N	12.36	144.39	117.20
1	D	286	ASP	CA-C-N	11.47	142.44	117.20
1	H	95	ALA	O-C-N	11.13	140.51	122.70
1	E	286	ASP	O-C-N	-11.05	105.02	122.70
1	D	81	GLY	CA-C-N	10.11	139.44	117.20
1	F	95	ALA	O-C-N	-10.05	106.63	122.70
1	F	81	GLY	CA-C-N	10.00	139.19	117.20
1	F	286	ASP	C-N-CA	9.05	144.33	121.70
1	H	95	ALA	CA-C-N	-8.86	97.72	117.20
1	H	285	ILE	CA-C-N	-8.83	97.77	117.20
1	E	194	ARG	O-C-N	-8.81	108.61	122.70
1	D	81	GLY	C-N-CA	8.80	143.71	121.70
1	H	71	CYS	O-C-N	8.75	138.07	123.20
1	F	81	GLY	C-N-CA	8.53	143.02	121.70
1	D	286	ASP	C-N-CA	8.44	142.79	121.70
1	C	273	ASP	O-C-N	-8.41	109.24	122.70
1	F	273	ASP	CA-C-N	8.38	135.64	117.20
1	A	94	MET	O-C-N	8.35	136.07	122.70
1	H	71	CYS	C-N-CA	-8.32	104.83	122.30
1	H	285	ILE	O-C-N	8.14	135.73	122.70
1	H	71	CYS	CA-C-N	-7.98	100.24	116.20
1	C	167	ARG	O-C-N	-7.88	110.09	122.70
1	A	287	LEU	C-N-CA	-7.80	105.92	122.30
1	H	285	ILE	C-N-CA	-7.53	102.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	45	SER	O-C-N	-7.43	110.82	122.70
1	C	286	ASP	CA-C-N	7.39	133.46	117.20
1	E	286	ASP	CA-C-N	7.34	133.36	117.20
1	F	273	ASP	C-N-CA	7.26	139.85	121.70
1	E	45	SER	O-C-N	7.16	134.15	122.70
1	A	287	LEU	O-C-N	7.14	135.34	123.20
1	E	46	TRP	O-C-N	-7.13	107.56	121.10
1	F	95	ALA	C-N-CA	7.06	139.34	121.70
1	D	273	ASP	O-C-N	-6.93	111.62	122.70
1	A	94	MET	C-N-CA	-6.88	104.50	121.70
1	E	273	ASP	O-C-N	-6.84	111.76	122.70
1	A	94	MET	CA-C-N	-6.75	102.35	117.20
1	F	95	ALA	CA-C-N	6.59	131.69	117.20
1	A	287	LEU	CA-C-N	-6.57	103.05	116.20
1	C	45	SER	O-C-N	-6.46	112.37	122.70
1	F	172	ILE	O-C-N	-6.32	112.59	122.70
1	H	95	ALA	C-N-CA	-6.25	106.08	121.70
1	D	44	VAL	O-C-N	-5.67	113.63	122.70
1	C	273	ASP	CA-C-N	5.59	129.49	117.20
1	B	157	PRO	O-C-N	5.56	131.60	122.70
1	C	167	ARG	CA-C-N	5.51	129.33	117.20
1	E	286	ASP	C-N-CA	5.51	135.46	121.70
1	E	194	ARG	CA-C-N	5.48	129.25	117.20
1	E	45	SER	CA-C-N	-5.46	105.19	117.20
1	E	45	SER	C-N-CA	-5.44	108.10	121.70
1	C	167	ARG	C-N-CA	5.42	135.25	121.70
1	C	286	ASP	C-N-CA	5.13	134.53	121.70
1	H	45	SER	CA-C-N	5.08	128.38	117.20
1	E	46	TRP	CA-C-N	5.08	131.32	117.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	150	ILE	Mainchain
1	C	286	ASP	Mainchain
1	E	95	ALA	Mainchain
1	F	273	ASP	Mainchain
1	F	286	ASP	Mainchain
1	F	71	CYS	Mainchain
1	F	81	GLY	Mainchain
1	G	82	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2206	0	2144	234	0
1	B	2205	0	2145	193	0
1	C	2205	0	2145	194	0
1	D	2214	0	2154	213	0
1	E	2209	0	2154	239	0
1	F	2209	0	2153	214	0
1	G	2205	0	2143	224	0
1	H	2208	0	2158	215	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	F	2	0	0	0	0
2	H	1	0	0	0	0
All	All	17667	0	17196	1571	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 45.

All (1571) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:C	1:A:288:GLY:CA	1.81	1.48
1:E:71:CYS:C	1:E:72:GLY:N	1.70	1.44
1:A:94:MET:C	1:A:95:ALA:CA	1.87	1.43
1:E:106:GLY:C	1:E:107:PRO:N	1.71	1.41
1:D:182:ARG:C	1:D:183:SER:N	1.70	1.40
1:A:287:LEU:CA	1:A:288:GLY:N	1.84	1.38
1:G:202:ARG:NH2	1:G:205:SER:HA	1.42	1.34
1:A:94:MET:CA	1:A:95:ALA:N	1.92	1.33
1:H:168:ILE:HD12	1:H:168:ILE:H	1.05	1.19
1:A:283:ARG:HE	1:D:23:ILE:CD1	1.55	1.19
1:F:93:THR:HG21	1:F:116:GLU:OE1	1.38	1.18
1:C:278:LEU:HD12	1:C:282:ARG:HG3	1.20	1.15
1:H:278:LEU:HD12	1:H:282:ARG:HG3	1.20	1.15
1:B:168:ILE:HD12	1:B:168:ILE:H	1.04	1.15
1:G:202:ARG:HH22	1:G:205:SER:CA	1.59	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ILE:H	1:E:168:ILE:HD12	1.05	1.14
1:D:168:ILE:H	1:D:168:ILE:HD12	1.05	1.14
1:G:202:ARG:NH2	1:G:205:SER:CA	2.11	1.13
1:A:278:LEU:HD12	1:A:282:ARG:HG3	1.20	1.13
1:G:168:ILE:H	1:G:168:ILE:HD12	1.04	1.13
1:B:278:LEU:HD12	1:B:282:ARG:HG3	1.20	1.12
1:A:168:ILE:H	1:A:168:ILE:HD12	1.06	1.12
1:F:278:LEU:HD12	1:F:282:ARG:HG3	1.20	1.12
1:A:287:LEU:O	1:A:288:GLY:N	1.84	1.11
1:D:278:LEU:HD12	1:D:282:ARG:HG3	1.20	1.11
1:G:278:LEU:HD12	1:G:282:ARG:HG3	1.20	1.10
1:E:278:LEU:HD12	1:E:282:ARG:HG3	1.20	1.09
1:F:168:ILE:H	1:F:168:ILE:HD12	1.05	1.09
1:A:283:ARG:HE	1:D:23:ILE:HD12	1.12	1.08
1:D:75:ILE:HD13	1:D:89:PHE:CD2	1.91	1.06
1:E:75:ILE:CD1	1:E:89:PHE:CD2	2.40	1.05
1:H:121:MET:SD	1:H:121:MET:N	2.30	1.05
1:G:202:ARG:HH21	1:G:205:SER:HB2	1.15	1.04
1:D:210:LEU:HD13	1:D:285:ILE:HD11	1.37	1.04
1:D:75:ILE:CD1	1:D:89:PHE:CD2	2.42	1.03
1:F:93:THR:CG2	1:F:116:GLU:OE1	2.07	1.01
1:F:75:ILE:CD1	1:F:89:PHE:CD2	2.43	1.00
1:A:94:MET:O	1:A:95:ALA:N	1.95	0.99
1:H:75:ILE:HD13	1:H:89:PHE:CD2	1.96	0.99
1:E:23:ILE:CD1	1:F:283:ARG:HE	1.74	0.98
1:F:75:ILE:HD13	1:F:89:PHE:CD2	1.99	0.98
1:B:75:ILE:HD13	1:B:89:PHE:CD2	1.98	0.97
1:E:76:GLU:HG2	1:E:105:ILE:HD11	1.46	0.96
1:E:75:ILE:HD13	1:E:89:PHE:CD2	2.00	0.96
1:C:280:ASP:OD2	1:C:282:ARG:HD3	1.66	0.96
1:A:287:LEU:O	1:A:288:GLY:CA	2.09	0.95
1:H:280:ASP:OD2	1:H:282:ARG:HD3	1.66	0.95
1:F:280:ASP:OD2	1:F:282:ARG:HD3	1.66	0.95
1:D:280:ASP:OD2	1:D:282:ARG:HD3	1.66	0.95
1:D:93:THR:HG21	1:D:116:GLU:OE1	1.66	0.95
1:B:280:ASP:OD2	1:B:282:ARG:HD3	1.66	0.94
1:A:280:ASP:OD2	1:A:282:ARG:HD3	1.66	0.94
1:E:75:ILE:HD11	1:E:89:PHE:CD2	2.02	0.94
1:G:280:ASP:OD2	1:G:282:ARG:HD3	1.66	0.94
1:E:61:ASN:HD21	1:E:94:MET:CE	1.81	0.94
1:C:75:ILE:HD13	1:C:89:PHE:CD2	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:CD1	1:B:89:PHE:CD2	2.51	0.94
1:B:61:ASN:HD21	1:B:94:MET:CE	1.80	0.94
1:G:75:ILE:HD13	1:G:89:PHE:CD2	2.02	0.93
1:A:283:ARG:HH21	1:D:23:ILE:HD11	1.34	0.93
1:C:75:ILE:CD1	1:C:89:PHE:CD2	2.51	0.93
1:E:280:ASP:OD2	1:E:282:ARG:HD3	1.66	0.92
1:E:23:ILE:HG21	1:F:285:ILE:HG13	1.50	0.92
1:H:121:MET:O	1:H:124:LEU:N	2.03	0.92
1:A:283:ARG:NE	1:D:23:ILE:CD1	2.32	0.92
1:A:94:MET:C	1:A:95:ALA:N	0.87	0.92
1:G:61:ASN:HD21	1:G:94:MET:CE	1.83	0.92
1:F:110:ASN:HB3	1:G:88:PHE:CD2	2.05	0.91
1:A:283:ARG:HH21	1:D:23:ILE:CD1	1.83	0.91
1:D:61:ASN:HD21	1:D:94:MET:CE	1.84	0.91
1:C:61:ASN:HD21	1:C:94:MET:CE	1.84	0.91
1:A:283:ARG:NE	1:D:23:ILE:HD12	1.87	0.90
1:B:61:ASN:HD21	1:B:94:MET:HE1	1.36	0.90
1:G:202:ARG:NH2	1:G:205:SER:CB	2.35	0.89
1:B:210:LEU:HD13	1:B:285:ILE:HD11	1.53	0.89
1:D:61:ASN:HD21	1:D:94:MET:HE1	1.38	0.89
1:H:168:ILE:CD1	1:H:168:ILE:H	1.81	0.89
1:E:168:ILE:CD1	1:E:168:ILE:H	1.81	0.88
1:F:168:ILE:H	1:F:168:ILE:CD1	1.81	0.88
1:G:210:LEU:HD13	1:G:285:ILE:HD11	1.53	0.88
1:G:202:ARG:HH21	1:G:205:SER:CB	1.86	0.88
1:E:56:LEU:O	1:E:60:THR:HG23	1.74	0.88
1:A:56:LEU:O	1:A:60:THR:HG23	1.74	0.88
1:A:94:MET:O	1:A:95:ALA:CA	2.21	0.88
1:B:56:LEU:O	1:B:60:THR:HG23	1.74	0.88
1:F:75:ILE:HD11	1:F:89:PHE:CD2	2.09	0.88
1:B:61:ASN:ND2	1:B:94:MET:HE1	1.88	0.88
1:B:168:ILE:CD1	1:B:168:ILE:H	1.81	0.87
1:G:202:ARG:NH2	1:G:205:SER:HB2	1.88	0.87
1:G:56:LEU:O	1:G:60:THR:HG23	1.74	0.87
1:E:93:THR:HG21	1:E:116:GLU:OE1	1.75	0.87
1:A:283:ARG:NH2	1:D:23:ILE:HD11	1.90	0.87
1:G:202:ARG:CZ	1:G:204:ARG:O	2.23	0.87
1:D:56:LEU:O	1:D:60:THR:HG23	1.74	0.87
1:G:93:THR:HG21	1:G:116:GLU:OE1	1.75	0.87
1:B:23:ILE:HG21	1:C:285:ILE:HG13	1.57	0.87
1:C:280:ASP:HB3	1:C:282:ARG:HG2	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:N	1:A:168:ILE:HD12	1.90	0.86
1:H:56:LEU:O	1:H:60:THR:HG23	1.74	0.86
1:D:44:VAL:CG1	1:D:48:VAL:HB	2.05	0.86
1:H:280:ASP:HB3	1:H:282:ARG:HG2	1.58	0.86
1:A:280:ASP:HB3	1:A:282:ARG:HG2	1.57	0.86
1:F:280:ASP:HB3	1:F:282:ARG:HG2	1.57	0.86
1:G:278:LEU:CD1	1:G:282:ARG:HG3	2.06	0.86
1:D:44:VAL:HG11	1:D:48:VAL:HG12	1.58	0.86
1:E:61:ASN:HD21	1:E:94:MET:HE1	1.40	0.86
1:E:280:ASP:HB3	1:E:282:ARG:HG2	1.57	0.86
1:F:56:LEU:O	1:F:60:THR:HG23	1.74	0.86
1:C:168:ILE:N	1:C:168:ILE:HD12	1.90	0.86
1:B:280:ASP:HB3	1:B:282:ARG:HG2	1.58	0.86
1:D:278:LEU:CD1	1:D:282:ARG:HG3	2.06	0.86
1:G:61:ASN:HD21	1:G:94:MET:HE1	1.40	0.86
1:H:172:ILE:HG13	1:H:246:HIS:HB3	1.57	0.86
1:E:168:ILE:N	1:E:168:ILE:HD12	1.90	0.85
1:C:56:LEU:O	1:C:60:THR:HG23	1.74	0.85
1:A:210:LEU:HD21	1:D:21:SER:OG	1.76	0.85
1:D:168:ILE:H	1:D:168:ILE:CD1	1.81	0.85
1:F:168:ILE:N	1:F:168:ILE:HD12	1.91	0.85
1:D:280:ASP:HB3	1:D:282:ARG:HG2	1.58	0.85
1:H:75:ILE:CD1	1:H:89:PHE:CD2	2.59	0.85
1:A:172:ILE:HG13	1:A:246:HIS:HB3	1.57	0.85
1:E:23:ILE:HD12	1:F:283:ARG:HE	1.39	0.84
1:E:172:ILE:HG13	1:E:246:HIS:HB3	1.57	0.84
1:G:280:ASP:HB3	1:G:282:ARG:HG2	1.57	0.84
1:B:93:THR:HG21	1:B:116:GLU:OE1	1.76	0.84
1:A:287:LEU:O	1:A:288:GLY:HA2	1.76	0.84
1:C:61:ASN:HD21	1:C:94:MET:HE1	1.40	0.84
1:A:61:ASN:HD21	1:A:94:MET:HE1	1.41	0.84
1:D:168:ILE:HD12	1:D:168:ILE:N	1.91	0.84
1:G:168:ILE:N	1:G:168:ILE:HD12	1.90	0.84
1:B:172:ILE:HG13	1:B:246:HIS:HB3	1.57	0.84
1:A:168:ILE:H	1:A:168:ILE:CD1	1.83	0.84
1:E:26:LEU:HB2	1:F:286:ASP:HA	1.58	0.84
1:D:172:ILE:HG13	1:D:246:HIS:HB3	1.57	0.84
1:E:278:LEU:CD1	1:E:282:ARG:HG3	2.06	0.83
1:G:172:ILE:HG13	1:G:246:HIS:HB3	1.57	0.83
1:G:202:ARG:NH2	1:G:204:ARG:O	2.11	0.83
1:B:168:ILE:HD12	1:B:168:ILE:N	1.90	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD13	1:A:89:PHE:CD2	2.14	0.83
1:F:172:ILE:HG13	1:F:246:HIS:HB3	1.57	0.83
1:C:278:LEU:HD12	1:C:282:ARG:CG	2.07	0.83
1:A:61:ASN:HD21	1:A:94:MET:CE	1.90	0.83
1:F:61:ASN:HD21	1:F:94:MET:CE	1.91	0.83
1:A:285:ILE:HG13	1:D:23:ILE:HG21	1.60	0.83
1:C:172:ILE:HG13	1:C:246:HIS:HB3	1.58	0.82
1:G:61:ASN:ND2	1:G:94:MET:HE1	1.94	0.82
1:F:278:LEU:HD12	1:F:282:ARG:CG	2.07	0.82
1:H:278:LEU:CD1	1:H:282:ARG:HG3	2.06	0.82
1:E:23:ILE:HD11	1:F:283:ARG:HH21	1.42	0.82
1:A:283:ARG:HE	1:D:23:ILE:HD11	1.45	0.82
1:F:278:LEU:CD1	1:F:282:ARG:HG3	2.06	0.81
1:B:273:ASP:OD1	1:B:274:VAL:N	2.13	0.81
1:H:61:ASN:HD21	1:H:94:MET:CE	1.93	0.81
1:A:278:LEU:CD1	1:A:282:ARG:HG3	2.06	0.81
1:D:210:LEU:HB3	1:D:285:ILE:HD13	1.63	0.81
1:A:283:ARG:HH21	1:D:23:ILE:CG1	1.93	0.81
1:C:278:LEU:CD1	1:C:282:ARG:HG3	2.06	0.81
1:E:278:LEU:HD12	1:E:282:ARG:CG	2.07	0.81
1:B:278:LEU:CD1	1:B:282:ARG:HG3	2.06	0.81
1:H:69:LEU:O	1:H:72:GLY:N	2.13	0.81
1:D:61:ASN:ND2	1:D:94:MET:HE1	1.95	0.81
1:D:75:ILE:HD11	1:D:89:PHE:CD2	2.14	0.80
1:G:210:LEU:HB3	1:G:285:ILE:CD1	2.11	0.80
1:G:278:LEU:HD12	1:G:282:ARG:CG	2.07	0.80
1:E:179:VAL:HG22	1:E:197:ASP:OD1	1.80	0.80
1:H:61:ASN:HD21	1:H:94:MET:HE1	1.47	0.80
1:H:168:ILE:HD12	1:H:168:ILE:N	1.90	0.80
1:H:278:LEU:HD12	1:H:282:ARG:CG	2.08	0.80
1:H:121:MET:O	1:H:122:LEU:C	2.11	0.80
1:A:287:LEU:C	1:A:288:GLY:N	0.75	0.79
1:E:75:ILE:HD13	1:E:89:PHE:CG	2.16	0.79
1:E:61:ASN:ND2	1:E:94:MET:HE1	1.96	0.79
1:B:61:ASN:ND2	1:B:94:MET:CE	2.44	0.79
1:B:201:THR:CG2	1:B:217:PRO:HD3	2.13	0.79
1:E:201:THR:CG2	1:E:217:PRO:HD3	2.13	0.79
1:D:201:THR:CG2	1:D:217:PRO:HD3	2.13	0.79
1:F:266:ILE:HG22	1:F:266:ILE:O	1.82	0.79
1:A:278:LEU:HD12	1:A:282:ARG:CG	2.07	0.79
1:D:278:LEU:HD12	1:D:282:ARG:CG	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:THR:CG2	1:C:217:PRO:HD3	2.13	0.79
1:E:23:ILE:CD1	1:F:283:ARG:HH21	1.95	0.78
1:G:23:ILE:HD11	1:H:283:ARG:HH11	1.46	0.78
1:G:201:THR:CG2	1:G:217:PRO:HD3	2.13	0.78
1:F:201:THR:CG2	1:F:217:PRO:HD3	2.13	0.78
1:A:201:THR:CG2	1:A:217:PRO:HD3	2.13	0.78
1:C:266:ILE:O	1:C:266:ILE:HG22	1.83	0.78
1:B:278:LEU:HD12	1:B:282:ARG:CG	2.08	0.78
1:C:61:ASN:ND2	1:C:94:MET:HE1	1.99	0.78
1:G:138:PRO:HB3	1:G:250:PHE:CD1	2.19	0.78
1:A:283:ARG:NE	1:D:23:ILE:HD11	1.99	0.78
1:D:266:ILE:HD12	1:D:293:ILE:HD12	1.65	0.78
1:D:138:PRO:HB3	1:D:250:PHE:CD1	2.19	0.78
1:H:266:ILE:HG22	1:H:266:ILE:O	1.83	0.78
1:G:168:ILE:H	1:G:168:ILE:CD1	1.81	0.77
1:B:138:PRO:HB3	1:B:250:PHE:CD1	2.19	0.77
1:H:201:THR:CG2	1:H:217:PRO:HD3	2.13	0.77
1:A:266:ILE:O	1:A:266:ILE:HG22	1.83	0.77
1:E:138:PRO:HB3	1:E:250:PHE:CD1	2.19	0.77
1:C:138:PRO:HB3	1:C:250:PHE:CD1	2.19	0.77
1:E:207:ILE:HD13	1:H:240:LEU:HD21	1.66	0.77
1:B:44:VAL:CG1	1:B:48:VAL:HB	2.14	0.77
1:H:138:PRO:HB3	1:H:250:PHE:CD1	2.19	0.77
1:F:138:PRO:HB3	1:F:250:PHE:CD1	2.19	0.77
1:D:266:ILE:HG22	1:D:266:ILE:O	1.82	0.77
1:F:44:VAL:CG1	1:F:48:VAL:HB	2.14	0.77
1:F:207:ILE:HG22	1:F:207:ILE:O	1.84	0.77
1:A:138:PRO:HB3	1:A:250:PHE:CD1	2.19	0.77
1:C:207:ILE:O	1:C:207:ILE:HG22	1.84	0.77
1:D:44:VAL:HG11	1:D:48:VAL:CG1	2.14	0.76
1:E:266:ILE:HG22	1:E:266:ILE:O	1.82	0.76
1:G:210:LEU:HB3	1:G:285:ILE:HD13	1.68	0.76
1:G:266:ILE:HG22	1:G:266:ILE:O	1.82	0.76
1:E:23:ILE:HD11	1:F:283:ARG:HE	1.51	0.76
1:B:207:ILE:O	1:B:207:ILE:HG22	1.84	0.76
1:B:266:ILE:HG22	1:B:266:ILE:O	1.83	0.76
1:F:210:LEU:HD13	1:F:285:ILE:HD11	1.66	0.76
1:G:23:ILE:HG21	1:H:285:ILE:HG13	1.67	0.76
1:D:104:PRO:HB2	1:D:110:ASN:OD1	1.85	0.76
1:C:75:ILE:HD11	1:C:89:PHE:CD2	2.20	0.76
1:F:93:THR:CG2	1:F:116:GLU:CD	2.54	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:ILE:HD12	1:G:293:ILE:HD12	1.68	0.76
1:G:207:ILE:O	1:G:207:ILE:HG22	1.84	0.76
1:A:207:ILE:O	1:A:207:ILE:HG22	1.84	0.76
1:F:75:ILE:HD11	1:F:89:PHE:CE2	2.19	0.75
1:G:202:ARG:HH22	1:G:205:SER:HA	0.69	0.75
1:D:74:VAL:HB	1:D:109:ALA:HB2	1.67	0.75
1:H:61:ASN:ND2	1:H:94:MET:HE1	2.01	0.75
1:D:210:LEU:HB3	1:D:285:ILE:CD1	2.17	0.75
1:F:266:ILE:HD12	1:F:293:ILE:HD12	1.68	0.75
1:D:207:ILE:O	1:D:207:ILE:HG22	1.85	0.75
1:D:93:THR:CG2	1:D:116:GLU:OE1	2.35	0.75
1:E:207:ILE:HG22	1:E:207:ILE:O	1.84	0.75
1:E:44:VAL:CG1	1:E:48:VAL:HB	2.17	0.74
1:H:207:ILE:O	1:H:207:ILE:HG22	1.84	0.74
1:H:266:ILE:HD12	1:H:293:ILE:HD12	1.68	0.74
1:A:266:ILE:HD12	1:A:293:ILE:HD12	1.68	0.74
1:E:272:VAL:CG1	1:E:273:ASP:N	2.51	0.74
1:G:44:VAL:CG1	1:G:48:VAL:HB	2.17	0.74
1:C:266:ILE:HD12	1:C:293:ILE:HD12	1.68	0.74
1:G:229:ASP:OD1	1:G:233:ARG:NH1	2.21	0.74
1:E:229:ASP:OD1	1:E:233:ARG:NH1	2.21	0.74
1:B:272:VAL:CG1	1:B:273:ASP:N	2.51	0.74
1:B:266:ILE:HD12	1:B:293:ILE:HD12	1.68	0.74
1:B:229:ASP:OD1	1:B:233:ARG:NH1	2.21	0.74
1:H:186:SER:OG	1:H:188:GLU:OE1	2.06	0.74
1:G:186:SER:OG	1:G:188:GLU:OE1	2.06	0.74
1:D:186:SER:OG	1:D:188:GLU:OE1	2.06	0.74
1:A:229:ASP:OD1	1:A:233:ARG:NH1	2.21	0.74
1:E:266:ILE:HD12	1:E:293:ILE:HD12	1.68	0.74
1:F:272:VAL:CG1	1:F:273:ASP:N	2.51	0.74
1:F:229:ASP:OD1	1:F:233:ARG:NH1	2.21	0.74
1:D:229:ASP:OD1	1:D:233:ARG:NH1	2.21	0.74
1:C:229:ASP:OD1	1:C:233:ARG:NH1	2.21	0.74
1:C:272:VAL:CG1	1:C:273:ASP:N	2.51	0.74
1:E:61:ASN:ND2	1:E:94:MET:CE	2.49	0.73
1:G:75:ILE:CD1	1:G:89:PHE:CD2	2.70	0.73
1:H:229:ASP:OD1	1:H:233:ARG:NH1	2.21	0.73
1:G:272:VAL:CG1	1:G:273:ASP:N	2.51	0.73
1:F:186:SER:OG	1:F:188:GLU:OE1	2.06	0.73
1:B:186:SER:OG	1:B:188:GLU:OE1	2.06	0.73
1:F:61:ASN:ND2	1:F:94:MET:HE1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:OG	1:A:188:GLU:OE1	2.06	0.73
1:D:61:ASN:ND2	1:D:94:MET:CE	2.51	0.73
1:F:185:ILE:CD1	1:F:191:VAL:HB	2.19	0.73
1:A:44:VAL:CG1	1:A:48:VAL:HB	2.19	0.73
1:C:185:ILE:CD1	1:C:191:VAL:HB	2.18	0.73
1:D:185:ILE:CD1	1:D:191:VAL:HB	2.19	0.73
1:D:44:VAL:HG13	1:D:48:VAL:HB	1.69	0.73
1:B:185:ILE:CD1	1:B:191:VAL:HB	2.18	0.73
1:D:272:VAL:CG1	1:D:273:ASP:N	2.51	0.73
1:G:185:ILE:CD1	1:G:191:VAL:HB	2.18	0.73
1:H:272:VAL:CG1	1:H:273:ASP:N	2.50	0.73
1:E:90:SER:O	1:E:93:THR:HG22	1.89	0.73
1:A:185:ILE:CD1	1:A:191:VAL:HB	2.18	0.73
1:A:90:SER:O	1:A:93:THR:HG22	1.89	0.73
1:B:90:SER:O	1:B:93:THR:HG22	1.89	0.73
1:E:185:ILE:CD1	1:E:191:VAL:HB	2.18	0.73
1:C:186:SER:OG	1:C:188:GLU:OE1	2.06	0.73
1:H:204:ARG:HH11	1:H:204:ARG:HG2	1.54	0.72
1:C:204:ARG:HH11	1:C:204:ARG:HG2	1.54	0.72
1:D:210:LEU:CD1	1:D:285:ILE:HD11	2.18	0.72
1:A:272:VAL:CG1	1:A:273:ASP:N	2.51	0.72
1:H:185:ILE:CD1	1:H:191:VAL:HB	2.18	0.72
1:F:204:ARG:HH11	1:F:204:ARG:HG2	1.55	0.72
1:A:94:MET:O	1:A:95:ALA:HA	1.88	0.72
1:D:75:ILE:HD11	1:D:89:PHE:CE2	2.24	0.72
1:E:186:SER:OG	1:E:188:GLU:OE1	2.06	0.72
1:A:283:ARG:NH2	1:D:23:ILE:CD1	2.50	0.72
1:E:23:ILE:CD1	1:F:283:ARG:NE	2.51	0.72
1:A:204:ARG:HH11	1:A:204:ARG:HG2	1.54	0.72
1:D:204:ARG:HH11	1:D:204:ARG:HG2	1.54	0.72
1:F:90:SER:O	1:F:93:THR:HG22	1.89	0.72
1:F:61:ASN:ND2	1:F:94:MET:CE	2.52	0.72
1:E:23:ILE:HD12	1:F:283:ARG:NE	2.05	0.72
1:D:44:VAL:CG1	1:D:48:VAL:CG1	2.68	0.72
1:H:94:MET:HB2	1:H:116:GLU:HG2	1.71	0.72
1:A:61:ASN:ND2	1:A:94:MET:HE1	2.03	0.72
1:G:61:ASN:ND2	1:G:94:MET:CE	2.49	0.72
1:B:204:ARG:HG2	1:B:204:ARG:HH11	1.54	0.72
1:G:204:ARG:HH11	1:G:204:ARG:HG2	1.55	0.71
1:D:75:ILE:CD1	1:D:89:PHE:CE2	2.72	0.71
1:C:61:ASN:ND2	1:C:94:MET:CE	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:THR:O	1:F:167:ARG:NH1	2.22	0.71
1:E:76:GLU:CG	1:E:105:ILE:HD11	2.20	0.71
1:F:75:ILE:HD13	1:F:89:PHE:CG	2.25	0.71
1:A:88:PHE:CD2	1:D:110:ASN:HB3	2.25	0.71
1:H:227:GLU:HG3	1:H:231:THR:OG1	1.90	0.71
1:D:90:SER:O	1:D:93:THR:HG22	1.89	0.71
1:C:90:SER:O	1:C:93:THR:HG22	1.89	0.71
1:G:227:GLU:HG3	1:G:231:THR:OG1	1.90	0.71
1:H:90:SER:O	1:H:93:THR:HG22	1.89	0.71
1:E:204:ARG:HH11	1:E:204:ARG:HG2	1.54	0.71
1:F:75:ILE:CD1	1:F:89:PHE:CE2	2.73	0.71
1:G:90:SER:O	1:G:93:THR:HG22	1.89	0.71
1:F:61:ASN:HD21	1:F:94:MET:HE1	1.55	0.71
1:B:75:ILE:HD11	1:B:89:PHE:CD2	2.25	0.71
1:F:227:GLU:HG3	1:F:231:THR:OG1	1.90	0.71
1:A:227:GLU:HG3	1:A:231:THR:OG1	1.90	0.71
1:C:227:GLU:HG3	1:C:231:THR:OG1	1.90	0.70
1:E:227:GLU:HG3	1:E:231:THR:OG1	1.90	0.70
1:H:200:LEU:HD13	1:H:214:VAL:CG1	2.21	0.70
1:A:274:VAL:HG12	1:A:289:LYS:HB2	1.74	0.70
1:D:227:GLU:HG3	1:D:231:THR:OG1	1.90	0.70
1:A:200:LEU:HD13	1:A:214:VAL:CG1	2.22	0.70
1:C:172:ILE:O	1:C:173:GLU:HB2	1.91	0.70
1:B:227:GLU:HG3	1:B:231:THR:OG1	1.90	0.70
1:H:127:ALA:O	1:H:131:ILE:HG12	1.92	0.70
1:D:200:LEU:HD13	1:D:214:VAL:CG1	2.21	0.70
1:A:287:LEU:C	1:A:288:GLY:HA2	2.03	0.70
1:A:287:LEU:N	1:A:288:GLY:N	2.39	0.70
1:D:75:ILE:HD13	1:D:89:PHE:CG	2.27	0.70
1:G:23:ILE:HD11	1:H:283:ARG:NH1	2.07	0.70
1:E:200:LEU:HD13	1:E:214:VAL:CG1	2.21	0.70
1:H:15:LEU:HD23	1:H:21:SER:HA	1.74	0.70
1:G:200:LEU:HD13	1:G:214:VAL:CG1	2.22	0.69
1:C:200:LEU:HD13	1:C:214:VAL:CG1	2.21	0.69
1:H:121:MET:O	1:H:123:GLY:N	2.24	0.69
1:A:184:GLU:OE1	1:A:194:ARG:HD2	1.93	0.69
1:D:18:ASP:O	1:D:257:ARG:NH1	2.24	0.69
1:A:283:ARG:CZ	1:D:23:ILE:HD11	2.22	0.69
1:E:99:TYR:OH	1:H:93:THR:OG1	2.03	0.69
1:B:200:LEU:HD13	1:B:214:VAL:CG1	2.22	0.69
1:D:127:ALA:O	1:D:131:ILE:HG12	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD23	1:A:21:SER:HA	1.74	0.69
1:H:261:SER:H	1:H:264:GLU:HG3	1.57	0.69
1:F:200:LEU:HD13	1:F:214:VAL:CG1	2.21	0.69
1:E:69:LEU:O	1:E:72:GLY:N	2.26	0.69
1:G:127:ALA:O	1:G:131:ILE:HG12	1.92	0.69
1:C:127:ALA:O	1:C:131:ILE:HG12	1.92	0.69
1:E:15:LEU:HD23	1:E:21:SER:HA	1.74	0.69
1:E:23:ILE:HD11	1:F:283:ARG:NH2	2.08	0.69
1:H:240:LEU:HD12	1:H:258:HIS:O	1.91	0.69
1:G:130:LEU:HD21	1:H:135:PHE:HE2	1.56	0.69
1:A:127:ALA:O	1:A:131:ILE:HG12	1.92	0.69
1:B:61:ASN:OD1	1:B:94:MET:HE2	1.93	0.69
1:F:127:ALA:O	1:F:131:ILE:HG12	1.92	0.69
1:B:139:THR:O	1:B:167:ARG:NH1	2.22	0.69
1:B:15:LEU:HD23	1:B:21:SER:HA	1.74	0.68
1:G:139:THR:O	1:G:167:ARG:NH1	2.22	0.68
1:G:15:LEU:HD23	1:G:21:SER:HA	1.74	0.68
1:H:139:THR:O	1:H:167:ARG:NH1	2.22	0.68
1:D:15:LEU:HD23	1:D:21:SER:HA	1.74	0.68
1:G:272:VAL:HG12	1:G:273:ASP:N	2.09	0.68
1:A:178:LEU:HD13	1:A:241:VAL:HG22	1.75	0.68
1:C:15:LEU:HD23	1:C:21:SER:HA	1.74	0.68
1:D:139:THR:O	1:D:167:ARG:NH1	2.22	0.68
1:A:272:VAL:HG12	1:A:273:ASP:N	2.08	0.68
1:D:178:LEU:HD13	1:D:241:VAL:HG22	1.75	0.68
1:A:132:TYR:HD1	1:D:129:SER:HB3	1.58	0.68
1:E:139:THR:O	1:E:167:ARG:NH1	2.22	0.68
1:C:210:LEU:HD13	1:C:285:ILE:HD11	1.75	0.68
1:H:273:ASP:OD1	1:H:274:VAL:N	2.27	0.68
1:B:178:LEU:HD13	1:B:241:VAL:HG22	1.75	0.68
1:H:178:LEU:HD13	1:H:241:VAL:HG22	1.75	0.68
1:D:104:PRO:CB	1:D:110:ASN:OD1	2.41	0.68
1:C:178:LEU:HD13	1:C:241:VAL:HG22	1.75	0.68
1:C:44:VAL:CG1	1:C:48:VAL:HB	2.24	0.68
1:D:272:VAL:HG12	1:D:273:ASP:N	2.08	0.68
1:E:127:ALA:O	1:E:131:ILE:HG12	1.92	0.68
1:E:178:LEU:HD13	1:E:241:VAL:HG22	1.75	0.68
1:F:272:VAL:HG12	1:F:273:ASP:N	2.08	0.67
1:B:127:ALA:O	1:B:131:ILE:HG12	1.92	0.67
1:D:14:ILE:HD13	1:D:14:ILE:N	2.10	0.67
1:E:272:VAL:HG12	1:E:273:ASP:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:VAL:HG12	1:H:273:ASP:N	2.08	0.67
1:G:178:LEU:HD13	1:G:241:VAL:HG22	1.75	0.67
1:A:14:ILE:HD13	1:A:14:ILE:N	2.10	0.67
1:A:91:VAL:HG21	1:D:114:THR:HG22	1.76	0.67
1:G:276:THR:HG22	1:G:277:THR:N	2.10	0.67
1:C:14:ILE:HD13	1:C:14:ILE:N	2.10	0.67
1:E:21:SER:OG	1:F:210:LEU:HD21	1.93	0.67
1:G:14:ILE:HD13	1:G:14:ILE:N	2.10	0.67
1:F:15:LEU:HD23	1:F:21:SER:HA	1.74	0.67
1:F:14:ILE:N	1:F:14:ILE:HD13	2.10	0.67
1:E:93:THR:CG2	1:E:116:GLU:OE1	2.42	0.67
1:B:272:VAL:HG12	1:B:273:ASP:N	2.08	0.66
1:C:272:VAL:HG12	1:C:273:ASP:N	2.08	0.66
1:F:240:LEU:HD12	1:F:258:HIS:O	1.96	0.66
1:B:276:THR:HG22	1:B:277:THR:N	2.10	0.66
1:D:276:THR:HG22	1:D:277:THR:N	2.10	0.66
1:C:240:LEU:HD12	1:C:258:HIS:O	1.95	0.66
1:H:44:VAL:CG1	1:H:48:VAL:HB	2.26	0.66
1:B:44:VAL:HG13	1:B:48:VAL:HB	1.76	0.66
1:F:276:THR:HG22	1:F:277:THR:N	2.10	0.66
1:H:276:THR:HG22	1:H:277:THR:N	2.10	0.66
1:C:276:THR:HG22	1:C:277:THR:N	2.10	0.66
1:D:104:PRO:CG	1:D:110:ASN:OD1	2.44	0.66
1:A:132:TYR:CD1	1:D:129:SER:HB3	2.31	0.66
1:A:240:LEU:HD12	1:A:258:HIS:O	1.96	0.66
1:B:14:ILE:HD13	1:B:14:ILE:N	2.10	0.66
1:A:276:THR:HG22	1:A:277:THR:N	2.10	0.66
1:H:14:ILE:HD13	1:H:14:ILE:N	2.10	0.66
1:A:210:LEU:HD13	1:A:285:ILE:HD11	1.78	0.66
1:E:94:MET:HB2	1:E:116:GLU:HG2	1.77	0.66
1:E:14:ILE:HD13	1:E:14:ILE:N	2.10	0.66
1:B:240:LEU:HD12	1:B:258:HIS:O	1.95	0.65
1:E:276:THR:HG22	1:E:277:THR:N	2.10	0.65
1:G:240:LEU:HD12	1:G:258:HIS:O	1.96	0.65
1:H:89:PHE:CD1	1:H:102:LEU:HB2	2.32	0.65
1:G:242:LEU:HD23	1:H:206:PRO:HB3	1.79	0.65
1:G:14:ILE:HG23	1:H:283:ARG:HH11	1.61	0.65
1:E:240:LEU:HD12	1:E:258:HIS:O	1.96	0.65
1:D:44:VAL:CG1	1:D:48:VAL:CB	2.74	0.65
1:G:273:ASP:OD1	1:G:274:VAL:N	2.29	0.65
1:D:240:LEU:HD12	1:D:258:HIS:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:SER:OG	1:H:210:LEU:HD21	1.95	0.65
1:C:139:THR:O	1:C:167:ARG:NH1	2.23	0.65
1:C:172:ILE:O	1:C:173:GLU:CB	2.43	0.65
1:E:179:VAL:CG2	1:E:197:ASP:OD1	2.44	0.65
1:C:240:LEU:HD21	1:D:207:ILE:HD13	1.77	0.65
1:G:41:LEU:O	1:G:134:ARG:NH1	2.30	0.65
1:A:139:THR:O	1:A:167:ARG:NH1	2.24	0.65
1:B:93:THR:CG2	1:B:116:GLU:OE1	2.44	0.65
1:C:93:THR:HG21	1:C:116:GLU:OE1	1.96	0.65
1:H:61:ASN:ND2	1:H:94:MET:CE	2.58	0.65
1:B:21:SER:OG	1:C:210:LEU:HD21	1.96	0.65
1:A:94:MET:N	1:A:95:ALA:N	2.45	0.65
1:C:75:ILE:HD13	1:C:89:PHE:CG	2.31	0.65
1:A:75:ILE:CD1	1:A:89:PHE:CD2	2.80	0.65
1:D:141:GLY:O	1:D:166:LEU:HB2	1.97	0.65
1:F:216:HIS:NE2	1:F:222:SER:OG	2.20	0.65
1:F:141:GLY:O	1:F:166:LEU:HB2	1.97	0.64
1:F:18:ASP:O	1:F:257:ARG:NH1	2.30	0.64
1:E:172:ILE:CG1	1:E:246:HIS:HB3	2.28	0.64
1:F:172:ILE:CG1	1:F:246:HIS:HB3	2.28	0.64
1:C:172:ILE:CG1	1:C:246:HIS:HB3	2.28	0.64
1:A:61:ASN:OD1	1:A:90:SER:OG	2.15	0.64
1:B:173:GLU:HA	1:B:206:PRO:HA	1.80	0.64
1:B:172:ILE:CG1	1:B:246:HIS:HB3	2.28	0.64
1:H:141:GLY:O	1:H:166:LEU:HB2	1.97	0.64
1:A:104:PRO:CG	1:A:110:ASN:OD1	2.45	0.64
1:G:141:GLY:O	1:G:166:LEU:HB2	1.97	0.64
1:D:94:MET:HB2	1:D:116:GLU:HG2	1.79	0.64
1:E:173:GLU:HA	1:E:206:PRO:HA	1.80	0.64
1:D:172:ILE:CG1	1:D:246:HIS:HB3	2.28	0.64
1:D:173:GLU:HA	1:D:206:PRO:HA	1.79	0.64
1:C:130:LEU:HD21	1:D:135:PHE:HE2	1.63	0.64
1:G:280:ASP:HB3	1:G:282:ARG:CG	2.28	0.64
1:G:172:ILE:CG1	1:G:246:HIS:HB3	2.28	0.64
1:G:173:GLU:HA	1:G:206:PRO:HA	1.80	0.64
1:H:93:THR:HG21	1:H:116:GLU:OE1	1.97	0.64
1:E:210:LEU:HB3	1:E:285:ILE:CD1	2.28	0.64
1:G:110:ASN:HB3	1:H:88:PHE:CD2	2.33	0.64
1:E:71:CYS:C	1:E:72:GLY:CA	2.65	0.64
1:G:89:PHE:CD1	1:G:102:LEU:HB2	2.32	0.64
1:B:44:VAL:HG11	1:B:48:VAL:HG12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ASP:OD1	1:E:39:HIS:HB3	1.98	0.64
1:G:94:MET:HB2	1:G:116:GLU:HG2	1.79	0.63
1:F:24:THR:O	1:G:284:ALA:HA	1.98	0.63
1:G:46:TRP:N	1:G:47:PRO:HD2	2.13	0.63
1:B:36:ASP:OD1	1:B:39:HIS:HB3	1.98	0.63
1:B:94:MET:HB2	1:B:116:GLU:HG2	1.80	0.63
1:F:173:GLU:O	1:F:173:GLU:HG3	1.98	0.63
1:H:88:PHE:O	1:H:92:GLN:HG3	1.99	0.63
1:F:44:VAL:HG13	1:F:48:VAL:HB	1.79	0.63
1:F:44:VAL:HG11	1:F:48:VAL:HG12	1.81	0.63
1:B:141:GLY:O	1:B:166:LEU:HB2	1.97	0.63
1:E:141:GLY:O	1:E:166:LEU:HB2	1.97	0.63
1:D:280:ASP:HB3	1:D:282:ARG:CG	2.28	0.63
1:B:88:PHE:O	1:B:92:GLN:HG3	1.99	0.63
1:F:178:LEU:HD13	1:F:241:VAL:HG22	1.79	0.63
1:F:280:ASP:HB3	1:F:282:ARG:CG	2.28	0.63
1:D:88:PHE:O	1:D:92:GLN:HG3	1.99	0.63
1:H:36:ASP:OD1	1:H:39:HIS:HB3	1.98	0.63
1:A:173:GLU:HA	1:A:206:PRO:HA	1.79	0.63
1:F:36:ASP:OD1	1:F:39:HIS:HB3	1.98	0.63
1:E:44:VAL:HG11	1:E:48:VAL:HG12	1.81	0.63
1:D:216:HIS:NE2	1:D:222:SER:OG	2.20	0.63
1:F:88:PHE:O	1:F:92:GLN:HG3	1.99	0.63
1:D:36:ASP:OD1	1:D:39:HIS:HB3	1.98	0.63
1:A:280:ASP:HB3	1:A:282:ARG:CG	2.28	0.63
1:A:89:PHE:CD1	1:A:102:LEU:HB2	2.32	0.63
1:A:36:ASP:OD1	1:A:39:HIS:HB3	1.98	0.63
1:A:88:PHE:O	1:A:92:GLN:HG3	1.99	0.63
1:A:261:SER:H	1:A:264:GLU:HG3	1.64	0.63
1:C:280:ASP:HB3	1:C:282:ARG:CG	2.28	0.63
1:E:88:PHE:O	1:E:92:GLN:HG3	1.99	0.63
1:B:261:SER:H	1:B:264:GLU:HG3	1.64	0.62
1:C:161:MET:HE2	1:C:162:ARG:N	2.14	0.62
1:E:261:SER:H	1:E:264:GLU:HG3	1.64	0.62
1:D:201:THR:HG22	1:D:217:PRO:HD3	1.81	0.62
1:H:182:ARG:HB3	1:H:237:SER:HB3	1.81	0.62
1:G:36:ASP:OD1	1:G:39:HIS:HB3	1.98	0.62
1:G:132:TYR:C	1:G:132:TYR:CD2	2.73	0.62
1:B:280:ASP:HB3	1:B:282:ARG:CG	2.28	0.62
1:H:173:GLU:HA	1:H:206:PRO:HA	1.80	0.62
1:D:173:GLU:HG3	1:D:173:GLU:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HG22	1:A:217:PRO:HD3	1.81	0.62
1:D:132:TYR:CD2	1:D:132:TYR:C	2.73	0.62
1:C:274:VAL:HG12	1:C:289:LYS:HB2	1.81	0.62
1:C:216:HIS:NE2	1:C:222:SER:OG	2.20	0.62
1:D:161:MET:HE2	1:D:162:ARG:N	2.14	0.62
1:H:173:GLU:O	1:H:173:GLU:HG3	1.98	0.62
1:E:173:GLU:HG3	1:E:173:GLU:O	1.98	0.62
1:F:201:THR:HG22	1:F:217:PRO:HD3	1.81	0.62
1:H:132:TYR:CD2	1:H:132:TYR:C	2.73	0.62
1:C:132:TYR:CD2	1:C:132:TYR:C	2.73	0.62
1:D:261:SER:H	1:D:264:GLU:HG3	1.64	0.62
1:C:36:ASP:OD1	1:C:39:HIS:HB3	1.98	0.62
1:E:132:TYR:C	1:E:132:TYR:CD2	2.73	0.62
1:G:201:THR:HG22	1:G:217:PRO:HD3	1.81	0.62
1:H:161:MET:HE2	1:H:162:ARG:N	2.15	0.62
1:E:61:ASN:OD1	1:E:90:SER:OG	2.17	0.62
1:G:93:THR:CG2	1:G:116:GLU:OE1	2.46	0.62
1:B:201:THR:HG22	1:B:217:PRO:HD3	1.81	0.62
1:G:14:ILE:HG23	1:H:283:ARG:NH1	2.14	0.62
1:G:261:SER:H	1:G:264:GLU:HG3	1.64	0.62
1:C:88:PHE:O	1:C:92:GLN:HG3	1.99	0.62
1:A:283:ARG:HH21	1:D:23:ILE:HG13	1.63	0.62
1:G:173:GLU:HG3	1:G:173:GLU:O	1.98	0.62
1:G:216:HIS:NE2	1:G:222:SER:OG	2.20	0.62
1:C:261:SER:H	1:C:264:GLU:HG3	1.64	0.62
1:C:201:THR:HG22	1:C:217:PRO:HD3	1.81	0.62
1:E:210:LEU:HD13	1:E:285:ILE:HD11	1.82	0.62
1:A:161:MET:HE2	1:A:162:ARG:N	2.15	0.62
1:F:261:SER:H	1:F:264:GLU:HG3	1.64	0.62
1:F:192:PHE:CE1	1:F:194:ARG:HB2	2.35	0.62
1:A:94:MET:C	1:A:95:ALA:HA	2.07	0.61
1:E:280:ASP:HB3	1:E:282:ARG:CG	2.28	0.61
1:B:173:GLU:O	1:B:173:GLU:HG3	1.98	0.61
1:G:88:PHE:O	1:G:92:GLN:HG3	1.99	0.61
1:H:201:THR:HG22	1:H:217:PRO:HD3	1.81	0.61
1:E:192:PHE:CE1	1:E:194:ARG:HB2	2.35	0.61
1:F:114:THR:HG22	1:G:91:VAL:HG21	1.81	0.61
1:A:182:ARG:HB3	1:A:237:SER:HB3	1.83	0.61
1:D:182:ARG:HB3	1:D:237:SER:HB3	1.83	0.61
1:A:173:GLU:HG3	1:A:173:GLU:O	1.98	0.61
1:E:201:THR:HG22	1:E:217:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:VAL:HG11	1:E:48:VAL:CG1	2.30	0.61
1:A:132:TYR:CD2	1:A:132:TYR:C	2.73	0.61
1:G:192:PHE:CE1	1:G:194:ARG:HB2	2.35	0.61
1:H:280:ASP:HB3	1:H:282:ARG:CG	2.28	0.61
1:E:23:ILE:CG1	1:F:283:ARG:HH21	2.14	0.61
1:B:132:TYR:CD2	1:B:132:TYR:C	2.73	0.61
1:H:158:THR:HG21	1:H:215:MET:HB3	1.83	0.61
1:H:172:ILE:CG1	1:H:246:HIS:HB3	2.28	0.61
1:C:182:ARG:HB3	1:C:237:SER:HB3	1.83	0.61
1:F:132:TYR:CD2	1:F:132:TYR:C	2.73	0.61
1:B:182:ARG:HB3	1:B:237:SER:HB3	1.83	0.61
1:C:158:THR:HG21	1:C:215:MET:HB3	1.83	0.61
1:A:158:THR:HG21	1:A:215:MET:HB3	1.83	0.61
1:C:153:PHE:CE2	1:C:154:GLU:OE1	2.54	0.61
1:D:153:PHE:CE2	1:D:154:GLU:OE1	2.54	0.61
1:A:283:ARG:CZ	1:D:23:ILE:CD1	2.79	0.60
1:B:158:THR:HG21	1:B:215:MET:HB3	1.83	0.60
1:B:216:HIS:NE2	1:B:222:SER:OG	2.20	0.60
1:F:158:THR:HG21	1:F:215:MET:HB3	1.83	0.60
1:E:153:PHE:CE2	1:E:154:GLU:OE1	2.54	0.60
1:D:158:THR:HG21	1:D:215:MET:HB3	1.83	0.60
1:E:88:PHE:CD2	1:H:110:ASN:HB3	2.35	0.60
1:E:158:THR:HG21	1:E:215:MET:HB3	1.83	0.60
1:F:153:PHE:CE2	1:F:154:GLU:OE1	2.54	0.60
1:H:69:LEU:O	1:H:72:GLY:CA	2.49	0.60
1:B:153:PHE:CE2	1:B:154:GLU:OE1	2.54	0.60
1:B:242:LEU:HD23	1:C:206:PRO:HB3	1.83	0.60
1:G:153:PHE:CE2	1:G:154:GLU:OE1	2.54	0.60
1:A:172:ILE:CG1	1:A:246:HIS:HB3	2.28	0.60
1:F:149:VAL:HG12	1:F:293:ILE:HD13	1.83	0.60
1:G:161:MET:HE2	1:G:162:ARG:N	2.16	0.60
1:E:161:MET:HE2	1:E:162:ARG:N	2.16	0.60
1:B:75:ILE:HD13	1:B:89:PHE:CG	2.36	0.60
1:H:149:VAL:HG12	1:H:293:ILE:HD13	1.83	0.60
1:G:46:TRP:O	1:G:47:PRO:C	2.39	0.60
1:A:153:PHE:CE2	1:A:154:GLU:OE1	2.54	0.60
1:G:158:THR:HG21	1:G:215:MET:HB3	1.83	0.60
1:A:69:LEU:O	1:A:72:GLY:N	2.35	0.60
1:G:149:VAL:HG12	1:G:293:ILE:HD13	1.83	0.60
1:A:41:LEU:O	1:A:134:ARG:NH1	2.34	0.60
1:E:149:VAL:HG12	1:E:293:ILE:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:LEU:O	1:H:72:GLY:HA2	2.02	0.59
1:H:153:PHE:CE2	1:H:154:GLU:OE1	2.54	0.59
1:B:161:MET:HE2	1:B:162:ARG:N	2.17	0.59
1:C:149:VAL:HG12	1:C:293:ILE:HD13	1.83	0.59
1:F:161:MET:HE2	1:F:162:ARG:N	2.18	0.59
1:B:149:VAL:HG12	1:B:293:ILE:HD13	1.83	0.59
1:E:23:ILE:CG2	1:F:285:ILE:HG13	2.26	0.59
1:C:295:GLN:C	1:E:292:GLU:HG2	2.22	0.59
1:C:104:PRO:HB2	1:C:110:ASN:OD1	2.02	0.59
1:A:216:HIS:NE2	1:A:222:SER:OG	2.20	0.59
1:F:110:ASN:C	1:G:88:PHE:CE2	2.75	0.58
1:F:110:ASN:HB3	1:G:88:PHE:CE2	2.38	0.58
1:B:192:PHE:CE1	1:B:194:ARG:HB2	2.38	0.58
1:F:93:THR:CG2	1:F:94:MET:N	2.67	0.58
1:D:93:THR:CG2	1:D:94:MET:N	2.67	0.58
1:F:110:ASN:CB	1:G:88:PHE:CE2	2.86	0.58
1:H:93:THR:CG2	1:H:94:MET:N	2.67	0.58
1:A:61:ASN:ND2	1:A:94:MET:CE	2.63	0.58
1:E:23:ILE:HD11	1:F:283:ARG:NE	2.16	0.58
1:B:44:VAL:HG11	1:B:48:VAL:CG1	2.33	0.58
1:G:110:ASN:HB3	1:H:88:PHE:CE2	2.38	0.58
1:A:26:LEU:HB2	1:B:285:ILE:O	2.04	0.58
1:F:44:VAL:HG11	1:F:48:VAL:CG1	2.33	0.58
1:E:216:HIS:NE2	1:E:222:SER:OG	2.20	0.58
1:F:94:MET:HB2	1:F:116:GLU:HG2	1.86	0.58
1:E:23:ILE:CD1	1:F:283:ARG:NH2	2.65	0.58
1:A:93:THR:CG2	1:A:94:MET:N	2.67	0.58
1:G:74:VAL:HB	1:G:109:ALA:HB2	1.86	0.58
1:G:274:VAL:HG12	1:G:289:LYS:HB2	1.85	0.58
1:E:93:THR:CG2	1:E:94:MET:N	2.67	0.57
1:G:93:THR:CG2	1:G:94:MET:N	2.67	0.57
1:A:110:ASN:O	1:A:114:THR:HG23	2.05	0.57
1:A:182:ARG:CB	1:A:237:SER:HB3	2.34	0.57
1:D:182:ARG:CB	1:D:237:SER:HB3	2.34	0.57
1:A:44:VAL:HG13	1:A:48:VAL:HB	1.85	0.57
1:C:110:ASN:O	1:C:114:THR:HG23	2.05	0.57
1:G:23:ILE:HD12	1:H:283:ARG:HB3	1.85	0.57
1:G:192:PHE:HE1	1:G:194:ARG:HB2	1.70	0.57
1:F:110:ASN:O	1:F:114:THR:HG23	2.05	0.57
1:H:185:ILE:CD1	1:H:191:VAL:CB	2.83	0.57
1:A:192:PHE:CE1	1:A:194:ARG:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASN:HB3	1:D:88:PHE:CD2	2.39	0.57
1:F:192:PHE:HE1	1:F:194:ARG:HB2	1.70	0.57
1:B:93:THR:CG2	1:B:94:MET:N	2.67	0.57
1:E:207:ILE:CD1	1:H:240:LEU:HD21	2.33	0.57
1:E:185:ILE:CD1	1:E:191:VAL:CB	2.83	0.57
1:A:74:VAL:HB	1:A:109:ALA:HB2	1.86	0.57
1:G:140:ALA:HB1	1:G:142:VAL:HG23	1.87	0.57
1:E:71:CYS:CA	1:E:72:GLY:N	2.63	0.57
1:D:110:ASN:O	1:D:114:THR:HG23	2.05	0.57
1:H:110:ASN:O	1:H:114:THR:HG23	2.05	0.57
1:G:110:ASN:O	1:G:114:THR:HG23	2.05	0.57
1:H:71:CYS:HB2	1:H:74:VAL:HG21	1.86	0.57
1:E:110:ASN:O	1:E:114:THR:HG23	2.05	0.56
1:G:44:VAL:HG11	1:G:48:VAL:CG1	2.35	0.56
1:A:185:ILE:CD1	1:A:191:VAL:CB	2.83	0.56
1:D:140:ALA:HB1	1:D:142:VAL:HG23	1.87	0.56
1:F:185:ILE:CD1	1:F:191:VAL:CB	2.83	0.56
1:B:210:LEU:HB3	1:B:285:ILE:HD13	1.87	0.56
1:D:185:ILE:CD1	1:D:191:VAL:CB	2.83	0.56
1:C:182:ARG:CB	1:C:237:SER:HB3	2.34	0.56
1:G:185:ILE:CD1	1:G:191:VAL:CB	2.83	0.56
1:A:140:ALA:HB1	1:A:142:VAL:HG23	1.87	0.56
1:F:274:VAL:HG12	1:F:289:LYS:HB2	1.87	0.56
1:C:93:THR:CG2	1:C:94:MET:N	2.67	0.56
1:B:185:ILE:CD1	1:B:191:VAL:CB	2.83	0.56
1:B:140:ALA:HB1	1:B:142:VAL:HG23	1.87	0.56
1:A:104:PRO:HB2	1:A:110:ASN:OD1	2.06	0.56
1:E:192:PHE:HE1	1:E:194:ARG:HB2	1.70	0.56
1:H:216:HIS:NE2	1:H:222:SER:OG	2.20	0.56
1:B:182:ARG:CB	1:B:237:SER:HB3	2.34	0.56
1:H:140:ALA:HB1	1:H:142:VAL:HG23	1.87	0.56
1:H:89:PHE:HD1	1:H:102:LEU:HB2	1.69	0.56
1:E:49:PHE:HE2	1:E:131:ILE:HD13	1.69	0.56
1:A:110:ASN:HB3	1:B:88:PHE:CD2	2.41	0.56
1:B:110:ASN:O	1:B:114:THR:HG23	2.05	0.56
1:F:140:ALA:HB1	1:F:142:VAL:HG23	1.87	0.56
1:E:95:ALA:C	1:E:96:THR:HG23	2.25	0.56
1:H:88:PHE:O	1:H:92:GLN:CG	2.55	0.55
1:G:130:LEU:O	1:G:134:ARG:HG2	2.06	0.55
1:E:140:ALA:HB1	1:E:142:VAL:HG23	1.87	0.55
1:E:26:LEU:HG	1:F:285:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:MET:HB2	1:C:116:GLU:HG2	1.88	0.55
1:E:130:LEU:O	1:E:134:ARG:HG2	2.06	0.55
1:D:116:GLU:O	1:D:117:ALA:C	2.45	0.55
1:B:116:GLU:O	1:B:117:ALA:C	2.45	0.55
1:A:88:PHE:O	1:A:92:GLN:CG	2.55	0.55
1:A:182:ARG:HA	1:A:193:ARG:NH1	2.20	0.55
1:F:55:GLY:O	1:F:59:VAL:HG23	2.07	0.55
1:G:175:ASP:OD1	1:G:175:ASP:C	2.45	0.55
1:F:61:ASN:OD1	1:F:94:MET:HE2	2.06	0.55
1:E:266:ILE:O	1:E:266:ILE:CG2	2.54	0.55
1:C:130:LEU:O	1:C:134:ARG:HG2	2.06	0.55
1:C:129:SER:HB3	1:D:132:TYR:CD1	2.42	0.55
1:A:240:LEU:HD21	1:B:207:ILE:HD13	1.88	0.55
1:H:175:ASP:OD1	1:H:175:ASP:C	2.45	0.55
1:D:175:ASP:OD1	1:D:175:ASP:C	2.45	0.55
1:A:130:LEU:O	1:A:134:ARG:HG2	2.06	0.55
1:C:140:ALA:HB1	1:C:142:VAL:HG23	1.87	0.55
1:G:55:GLY:O	1:G:59:VAL:HG23	2.07	0.55
1:B:69:LEU:O	1:B:72:GLY:N	2.39	0.55
1:F:116:GLU:O	1:F:117:ALA:C	2.45	0.55
1:A:201:THR:HG22	1:A:217:PRO:CD	2.37	0.55
1:E:227:GLU:OE2	1:E:231:THR:HB	2.07	0.55
1:E:132:TYR:CD1	1:H:129:SER:HB3	2.42	0.55
1:B:55:GLY:O	1:B:59:VAL:HG23	2.07	0.55
1:C:55:GLY:O	1:C:59:VAL:HG23	2.07	0.55
1:C:185:ILE:CD1	1:C:191:VAL:CB	2.83	0.55
1:A:175:ASP:C	1:A:175:ASP:OD1	2.45	0.55
1:E:88:PHE:O	1:E:92:GLN:CG	2.55	0.55
1:H:201:THR:HG22	1:H:217:PRO:CD	2.37	0.55
1:E:44:VAL:HG13	1:E:48:VAL:HB	1.87	0.55
1:C:175:ASP:OD1	1:C:175:ASP:C	2.45	0.55
1:F:130:LEU:O	1:F:134:ARG:HG2	2.06	0.55
1:F:175:ASP:C	1:F:175:ASP:OD1	2.45	0.55
1:H:130:LEU:O	1:H:134:ARG:HG2	2.06	0.55
1:B:88:PHE:O	1:B:92:GLN:CG	2.55	0.55
1:D:88:PHE:O	1:D:92:GLN:CG	2.55	0.55
1:A:55:GLY:O	1:A:59:VAL:HG23	2.07	0.55
1:H:172:ILE:O	1:H:173:GLU:HG2	2.07	0.55
1:A:172:ILE:O	1:A:173:GLU:HG2	2.07	0.55
1:D:172:ILE:O	1:D:173:GLU:HG2	2.07	0.55
1:H:116:GLU:O	1:H:117:ALA:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:THR:HG22	1:B:217:PRO:CD	2.37	0.55
1:D:201:THR:HG22	1:D:217:PRO:CD	2.37	0.55
1:B:266:ILE:CG2	1:B:266:ILE:O	2.54	0.55
1:D:210:LEU:HD22	1:D:285:ILE:CD1	2.37	0.54
1:G:172:ILE:O	1:G:173:GLU:HG2	2.07	0.54
1:C:201:THR:HG22	1:C:217:PRO:CD	2.37	0.54
1:H:138:PRO:HB3	1:H:250:PHE:CG	2.42	0.54
1:G:227:GLU:OE2	1:G:231:THR:HB	2.07	0.54
1:B:227:GLU:OE2	1:B:231:THR:HB	2.07	0.54
1:E:88:PHE:CE2	1:H:110:ASN:HB3	2.42	0.54
1:B:192:PHE:HE1	1:B:194:ARG:HB2	1.72	0.54
1:G:89:PHE:HB2	1:G:102:LEU:HD13	1.88	0.54
1:C:116:GLU:O	1:C:117:ALA:C	2.45	0.54
1:H:61:ASN:OD1	1:H:94:MET:HE2	2.08	0.54
1:E:201:THR:HG22	1:E:217:PRO:CD	2.37	0.54
1:H:227:GLU:OE2	1:H:231:THR:HB	2.07	0.54
1:B:130:LEU:O	1:B:134:ARG:HG2	2.06	0.54
1:D:55:GLY:O	1:D:59:VAL:HG23	2.07	0.54
1:E:110:ASN:HB3	1:F:88:PHE:CD2	2.43	0.54
1:E:26:LEU:HD12	1:F:286:ASP:HB2	1.90	0.54
1:G:61:ASN:OD1	1:G:90:SER:OG	2.25	0.54
1:G:88:PHE:O	1:G:92:GLN:CG	2.55	0.54
1:A:227:GLU:OE2	1:A:231:THR:HB	2.07	0.54
1:D:130:LEU:O	1:D:134:ARG:HG2	2.06	0.54
1:C:49:PHE:HE2	1:C:131:ILE:HD13	1.72	0.54
1:A:283:ARG:NH2	1:D:23:ILE:HG13	2.22	0.54
1:E:175:ASP:C	1:E:175:ASP:OD1	2.45	0.54
1:G:49:PHE:HE2	1:G:131:ILE:HD13	1.73	0.54
1:E:210:LEU:HB3	1:E:285:ILE:HD11	1.89	0.54
1:C:88:PHE:O	1:C:92:GLN:CG	2.55	0.54
1:C:184:GLU:OE1	1:C:194:ARG:HD2	2.07	0.54
1:B:209:SER:O	1:B:210:LEU:HD23	2.08	0.54
1:F:201:THR:HG22	1:F:217:PRO:CD	2.37	0.54
1:F:138:PRO:HB3	1:F:250:PHE:CG	2.42	0.54
1:B:175:ASP:C	1:B:175:ASP:OD1	2.45	0.54
1:D:46:TRP:O	1:D:50:ILE:HG13	2.08	0.54
1:G:210:LEU:HB3	1:G:285:ILE:HD11	1.90	0.54
1:C:209:SER:O	1:C:210:LEU:HD23	2.08	0.54
1:B:172:ILE:O	1:B:173:GLU:HG2	2.07	0.54
1:A:138:PRO:HB3	1:A:250:PHE:CG	2.42	0.54
1:H:182:ARG:CB	1:H:237:SER:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:GLY:O	1:H:59:VAL:HG23	2.07	0.54
1:A:116:GLU:O	1:A:117:ALA:C	2.45	0.54
1:F:88:PHE:O	1:F:92:GLN:CG	2.55	0.54
1:D:61:ASN:OD1	1:D:94:MET:HE2	2.08	0.54
1:G:201:THR:HG22	1:G:217:PRO:CD	2.37	0.54
1:E:55:GLY:O	1:E:59:VAL:HG23	2.07	0.54
1:E:116:GLU:O	1:E:117:ALA:C	2.45	0.54
1:D:44:VAL:HG13	1:D:48:VAL:CB	2.35	0.54
1:E:138:PRO:HB3	1:E:250:PHE:CG	2.42	0.54
1:D:276:THR:CG2	1:D:277:THR:N	2.71	0.54
1:C:276:THR:CG2	1:C:277:THR:N	2.71	0.54
1:E:209:SER:O	1:E:210:LEU:HD23	2.08	0.54
1:F:209:SER:O	1:F:210:LEU:HD23	2.08	0.54
1:B:149:VAL:CG1	1:B:293:ILE:HD13	2.38	0.54
1:E:132:TYR:HD1	1:H:129:SER:HB3	1.73	0.54
1:C:46:TRP:O	1:C:50:ILE:HG13	2.08	0.54
1:A:209:SER:O	1:A:210:LEU:HD23	2.08	0.54
1:C:172:ILE:O	1:C:173:GLU:C	2.41	0.54
1:H:149:VAL:CG1	1:H:293:ILE:HD13	2.38	0.54
1:D:227:GLU:OE2	1:D:231:THR:HB	2.07	0.54
1:E:49:PHE:CE2	1:E:131:ILE:HD13	2.43	0.54
1:B:276:THR:CG2	1:B:277:THR:N	2.71	0.54
1:A:276:THR:CG2	1:A:277:THR:N	2.71	0.54
1:C:295:GLN:O	1:E:292:GLU:HG2	2.07	0.54
1:C:138:PRO:HB3	1:C:250:PHE:CG	2.42	0.53
1:E:207:ILE:CG2	1:E:207:ILE:O	2.56	0.53
1:F:276:THR:CG2	1:F:277:THR:N	2.71	0.53
1:B:46:TRP:O	1:B:50:ILE:HG13	2.08	0.53
1:E:172:ILE:O	1:E:173:GLU:HG2	2.07	0.53
1:A:138:PRO:CG	1:A:252:GLN:OE1	2.56	0.53
1:F:227:GLU:OE2	1:F:231:THR:HB	2.07	0.53
1:C:227:GLU:OE2	1:C:231:THR:HB	2.07	0.53
1:H:276:THR:CG2	1:H:277:THR:N	2.71	0.53
1:H:182:ARG:HB3	1:H:237:SER:CB	2.39	0.53
1:B:138:PRO:HB3	1:B:250:PHE:CG	2.42	0.53
1:E:149:VAL:CG1	1:E:293:ILE:HD13	2.38	0.53
1:G:40:ASP:O	1:G:44:VAL:HG23	2.09	0.53
1:G:276:THR:CG2	1:G:277:THR:N	2.71	0.53
1:E:276:THR:CG2	1:E:277:THR:N	2.71	0.53
1:G:138:PRO:HB3	1:G:250:PHE:CG	2.42	0.53
1:C:240:LEU:HD21	1:D:207:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:VAL:HG13	1:G:48:VAL:HB	1.90	0.53
1:A:283:ARG:HB3	1:D:23:ILE:HD12	1.91	0.53
1:E:75:ILE:HD11	1:E:89:PHE:HD2	1.70	0.53
1:F:149:VAL:CG1	1:F:293:ILE:HD13	2.38	0.53
1:H:209:SER:O	1:H:210:LEU:HD23	2.08	0.53
1:F:40:ASP:O	1:F:44:VAL:HG23	2.09	0.53
1:G:149:VAL:CG1	1:G:293:ILE:HD13	2.38	0.53
1:A:207:ILE:CG2	1:A:207:ILE:O	2.56	0.53
1:A:44:VAL:HG11	1:A:48:VAL:HG12	1.90	0.53
1:A:46:TRP:O	1:A:50:ILE:HG13	2.08	0.53
1:H:46:TRP:O	1:H:50:ILE:HG13	2.08	0.53
1:G:209:SER:O	1:G:210:LEU:HD23	2.08	0.53
1:D:138:PRO:HB3	1:D:250:PHE:CG	2.42	0.53
1:B:207:ILE:O	1:B:207:ILE:CG2	2.56	0.53
1:C:192:PHE:CE1	1:C:194:ARG:HB2	2.44	0.53
1:D:209:SER:O	1:D:210:LEU:HD23	2.08	0.53
1:D:40:ASP:O	1:D:44:VAL:HG23	2.09	0.53
1:C:149:VAL:CG1	1:C:293:ILE:HD13	2.38	0.53
1:A:40:ASP:O	1:A:44:VAL:HG23	2.09	0.53
1:C:41:LEU:O	1:C:134:ARG:NH1	2.38	0.53
1:E:130:LEU:HD21	1:F:135:PHE:HE2	1.74	0.53
1:G:116:GLU:O	1:G:117:ALA:C	2.45	0.53
1:C:40:ASP:O	1:C:44:VAL:HG23	2.09	0.53
1:H:40:ASP:O	1:H:44:VAL:HG23	2.09	0.53
1:B:74:VAL:HB	1:B:109:ALA:HB2	1.91	0.53
1:C:26:LEU:HB2	1:D:285:ILE:O	2.09	0.52
1:B:210:LEU:HB3	1:B:285:ILE:CD1	2.39	0.52
1:B:40:ASP:O	1:B:44:VAL:HG23	2.09	0.52
1:G:44:VAL:HG11	1:G:48:VAL:HG12	1.90	0.52
1:A:192:PHE:HE1	1:A:194:ARG:HB2	1.74	0.52
1:F:74:VAL:HB	1:F:109:ALA:HB2	1.91	0.52
1:C:299:HIS:HA	1:E:147:ARG:HH22	1.74	0.52
1:E:75:ILE:HD11	1:E:89:PHE:CE2	2.44	0.52
1:E:15:LEU:HB2	1:E:238:GLU:OE1	2.08	0.52
1:G:61:ASN:OD1	1:G:94:MET:HE2	2.09	0.52
1:C:44:VAL:HG13	1:C:48:VAL:HB	1.88	0.52
1:B:15:LEU:HB2	1:B:238:GLU:OE1	2.09	0.52
1:C:182:ARG:HB3	1:C:237:SER:CB	2.40	0.52
1:D:182:ARG:HB3	1:D:237:SER:CB	2.40	0.52
1:B:185:ILE:HD11	1:B:191:VAL:HB	1.92	0.52
1:B:182:ARG:HB3	1:B:237:SER:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:HD12	1:G:60:THR:HG23	1.92	0.52
1:F:34:LEU:HG	1:F:34:LEU:O	2.09	0.52
1:C:61:ASN:OD1	1:C:90:SER:OG	2.24	0.52
1:G:49:PHE:CE2	1:G:131:ILE:HD13	2.45	0.52
1:A:182:ARG:HB3	1:A:237:SER:CB	2.40	0.52
1:G:129:SER:HB3	1:H:132:TYR:CD1	2.45	0.51
1:G:129:SER:HB3	1:H:132:TYR:HD1	1.74	0.51
1:F:110:ASN:CB	1:G:88:PHE:CD2	2.87	0.51
1:C:56:LEU:HD12	1:C:60:THR:HG23	1.92	0.51
1:E:158:THR:HG23	1:E:216:HIS:C	2.31	0.51
1:F:44:VAL:CG1	1:F:48:VAL:CG1	2.88	0.51
1:E:40:ASP:O	1:E:44:VAL:HG23	2.09	0.51
1:B:158:THR:HG23	1:B:216:HIS:C	2.31	0.51
1:D:56:LEU:HD12	1:D:60:THR:HG23	1.92	0.51
1:F:272:VAL:HG13	1:F:273:ASP:H	1.75	0.51
1:B:23:ILE:CG2	1:C:285:ILE:HG13	2.35	0.51
1:C:158:THR:HG23	1:C:216:HIS:C	2.31	0.51
1:F:185:ILE:HD11	1:F:191:VAL:HB	1.92	0.51
1:A:44:VAL:HG11	1:A:48:VAL:CG1	2.40	0.51
1:C:106:GLY:O	1:C:110:ASN:ND2	2.44	0.51
1:A:104:PRO:CB	1:A:110:ASN:OD1	2.58	0.51
1:H:192:PHE:CE1	1:H:194:ARG:HB2	2.45	0.51
1:E:219:ASP:OD1	1:E:219:ASP:C	2.49	0.51
1:G:56:LEU:HD12	1:G:56:LEU:O	2.11	0.51
1:F:158:THR:HG23	1:F:216:HIS:C	2.31	0.51
1:C:272:VAL:HG13	1:C:273:ASP:H	1.75	0.51
1:A:158:THR:HG23	1:A:216:HIS:C	2.31	0.51
1:G:18:ASP:O	1:G:257:ARG:NH1	2.43	0.51
1:E:56:LEU:HD12	1:E:56:LEU:O	2.11	0.51
1:B:44:VAL:CG1	1:B:48:VAL:CB	2.88	0.51
1:E:44:VAL:CG1	1:E:48:VAL:CG1	2.89	0.51
1:G:200:LEU:HD13	1:G:214:VAL:HG12	1.92	0.51
1:C:49:PHE:CE2	1:C:131:ILE:HD13	2.45	0.51
1:A:49:PHE:HE2	1:A:131:ILE:HD13	1.76	0.51
1:D:158:THR:HG23	1:D:216:HIS:C	2.31	0.51
1:B:104:PRO:HB2	1:B:110:ASN:OD1	2.11	0.51
1:H:158:THR:HG23	1:H:216:HIS:C	2.31	0.51
1:E:147:ARG:NH1	1:E:147:ARG:HG2	2.26	0.51
1:B:147:ARG:NH1	1:B:147:ARG:HG2	2.26	0.51
1:F:42:LEU:HB3	1:F:137:ARG:NH2	2.26	0.51
1:D:56:LEU:HD12	1:D:56:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:LEU:HD12	1:H:60:THR:HG23	1.92	0.51
1:A:147:ARG:HG2	1:A:147:ARG:NH1	2.26	0.51
1:E:185:ILE:HD11	1:E:191:VAL:HB	1.92	0.51
1:A:114:THR:HG22	1:B:91:VAL:HG21	1.93	0.51
1:G:158:THR:HG23	1:G:216:HIS:C	2.31	0.51
1:A:219:ASP:OD1	1:A:219:ASP:C	2.49	0.51
1:A:210:LEU:HB3	1:A:285:ILE:CD1	2.42	0.50
1:F:94:MET:HB2	1:F:116:GLU:CG	2.41	0.50
1:C:56:LEU:O	1:C:56:LEU:HD12	2.11	0.50
1:B:44:VAL:CG1	1:B:48:VAL:CG1	2.90	0.50
1:G:184:GLU:OE1	1:G:194:ARG:HD2	2.11	0.50
1:A:18:ASP:O	1:A:257:ARG:NH1	2.44	0.50
1:E:156:LYS:O	1:E:157:PRO:C	2.46	0.50
1:H:147:ARG:NH1	1:H:147:ARG:HG2	2.26	0.50
1:D:266:ILE:HG22	1:D:269:GLY:HA3	1.94	0.50
1:H:272:VAL:HG13	1:H:273:ASP:H	1.75	0.50
1:E:170:GLN:HE22	1:H:21:SER:H	1.59	0.50
1:B:56:LEU:O	1:B:56:LEU:HD12	2.11	0.50
1:D:147:ARG:HG2	1:D:147:ARG:NH1	2.26	0.50
1:A:272:VAL:HG13	1:A:273:ASP:H	1.75	0.50
1:A:56:LEU:HD12	1:A:60:THR:HG23	1.92	0.50
1:B:272:VAL:HG13	1:B:273:ASP:H	1.75	0.50
1:B:110:ASN:O	1:B:113:VAL:HB	2.12	0.50
1:C:147:ARG:NH1	1:C:147:ARG:HG2	2.26	0.50
1:B:219:ASP:OD1	1:B:219:ASP:C	2.49	0.50
1:E:110:ASN:O	1:E:113:VAL:HB	2.12	0.50
1:D:61:ASN:OD1	1:D:90:SER:OG	2.25	0.50
1:D:44:VAL:HG13	1:D:48:VAL:CG1	2.41	0.50
1:A:89:PHE:HD1	1:A:102:LEU:HB2	1.77	0.50
1:G:23:ILE:CD1	1:H:283:ARG:HB3	2.41	0.50
1:A:91:VAL:HG21	1:D:114:THR:CG2	2.42	0.50
1:E:272:VAL:HG13	1:E:273:ASP:H	1.75	0.50
1:F:272:VAL:CG1	1:F:273:ASP:H	2.25	0.50
1:C:204:ARG:NH1	1:C:204:ARG:HG2	2.25	0.50
1:B:280:ASP:O	1:B:280:ASP:OD1	2.30	0.50
1:B:56:LEU:HD12	1:B:60:THR:HG23	1.92	0.50
1:F:172:ILE:O	1:F:173:GLU:HG2	2.11	0.50
1:A:44:VAL:CG1	1:A:45:SER:N	2.75	0.50
1:H:185:ILE:HD11	1:H:191:VAL:HB	1.92	0.50
1:A:204:ARG:NH1	1:A:204:ARG:HG2	2.25	0.50
1:E:200:LEU:HD13	1:E:214:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:GLU:OE1	1:E:194:ARG:HD2	2.11	0.50
1:B:18:ASP:O	1:B:257:ARG:NH1	2.45	0.50
1:H:219:ASP:C	1:H:219:ASP:OD1	2.49	0.50
1:E:280:ASP:OD1	1:E:280:ASP:O	2.30	0.50
1:B:116:GLU:O	1:B:119:CYS:N	2.45	0.50
1:F:110:ASN:O	1:F:113:VAL:HB	2.12	0.50
1:H:116:GLU:O	1:H:119:CYS:N	2.45	0.50
1:G:201:THR:HG23	1:G:217:PRO:HD3	1.93	0.50
1:F:204:ARG:NH1	1:F:204:ARG:HG2	2.25	0.50
1:C:219:ASP:OD1	1:C:219:ASP:C	2.49	0.50
1:F:219:ASP:OD1	1:F:219:ASP:C	2.49	0.50
1:G:147:ARG:HG2	1:G:147:ARG:NH1	2.26	0.50
1:A:116:GLU:O	1:A:119:CYS:N	2.45	0.50
1:F:104:PRO:HB2	1:F:110:ASN:OD1	2.11	0.50
1:E:56:LEU:HD12	1:E:60:THR:HG23	1.92	0.50
1:D:147:ARG:HB2	1:D:293:ILE:HD11	1.94	0.50
1:F:200:LEU:HD13	1:F:214:VAL:HG12	1.92	0.50
1:F:184:GLU:OE1	1:F:194:ARG:HD2	2.11	0.50
1:H:56:LEU:O	1:H:56:LEU:HD12	2.11	0.50
1:F:56:LEU:HD12	1:F:60:THR:HG23	1.92	0.50
1:A:88:PHE:CE2	1:D:110:ASN:CB	2.95	0.50
1:D:104:PRO:HB2	1:D:110:ASN:CG	2.31	0.50
1:G:272:VAL:HG13	1:G:273:ASP:H	1.75	0.50
1:D:272:VAL:HG13	1:D:273:ASP:H	1.75	0.50
1:C:44:VAL:CG1	1:C:45:SER:N	2.75	0.50
1:C:110:ASN:O	1:C:113:VAL:HB	2.12	0.50
1:F:129:SER:HB3	1:G:132:TYR:CD1	2.47	0.50
1:A:56:LEU:HD12	1:A:56:LEU:O	2.11	0.49
1:H:44:VAL:CG1	1:H:45:SER:N	2.74	0.49
1:C:280:ASP:O	1:C:280:ASP:OD1	2.30	0.49
1:H:280:ASP:OD1	1:H:280:ASP:O	2.30	0.49
1:E:75:ILE:O	1:E:76:GLU:O	2.28	0.49
1:B:75:ILE:CD1	1:B:89:PHE:CE2	2.95	0.49
1:E:61:ASN:HD21	1:E:94:MET:HE2	1.72	0.49
1:G:110:ASN:O	1:G:113:VAL:HB	2.12	0.49
1:G:116:GLU:O	1:G:119:CYS:N	2.45	0.49
1:F:56:LEU:HD12	1:F:56:LEU:O	2.11	0.49
1:G:15:LEU:HB2	1:G:238:GLU:OE1	2.12	0.49
1:C:272:VAL:CG1	1:C:273:ASP:H	2.25	0.49
1:A:110:ASN:O	1:A:113:VAL:HB	2.12	0.49
1:E:210:LEU:HB3	1:E:285:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:GLU:HB2	1:G:247:HIS:HE1	1.77	0.49
1:E:46:TRP:N	1:E:47:PRO:HD2	2.27	0.49
1:F:147:ARG:HG2	1:F:147:ARG:NH1	2.26	0.49
1:H:54:THR:O	1:H:57:TYR:HB3	2.13	0.49
1:D:280:ASP:OD1	1:D:280:ASP:O	2.30	0.49
1:G:44:VAL:CG1	1:G:45:SER:N	2.75	0.49
1:D:54:THR:O	1:D:57:TYR:HB3	2.13	0.49
1:C:76:GLU:HG3	1:C:77:ASN:ND2	2.28	0.49
1:B:169:GLU:HB2	1:B:247:HIS:HE1	1.77	0.49
1:H:76:GLU:HG3	1:H:77:ASN:ND2	2.28	0.49
1:A:76:GLU:HG3	1:A:77:ASN:ND2	2.28	0.49
1:H:168:ILE:CD1	1:H:168:ILE:N	2.61	0.49
1:G:280:ASP:OD1	1:G:280:ASP:O	2.30	0.49
1:D:116:GLU:O	1:D:119:CYS:N	2.45	0.49
1:B:200:LEU:HD13	1:B:214:VAL:HG12	1.92	0.49
1:B:153:PHE:O	1:B:154:GLU:C	2.50	0.49
1:G:153:PHE:O	1:G:154:GLU:C	2.50	0.49
1:D:76:GLU:HG3	1:D:77:ASN:ND2	2.28	0.49
1:D:169:GLU:HB2	1:D:247:HIS:HE1	1.77	0.49
1:C:54:THR:O	1:C:57:TYR:HB3	2.13	0.49
1:F:169:GLU:HB2	1:F:247:HIS:HE1	1.77	0.49
1:A:54:THR:O	1:A:57:TYR:HB3	2.13	0.49
1:E:106:GLY:O	1:E:110:ASN:ND2	2.44	0.49
1:B:61:ASN:CG	1:B:94:MET:HE2	2.33	0.49
1:F:44:VAL:CG1	1:F:48:VAL:CB	2.88	0.49
1:H:204:ARG:NH1	1:H:204:ARG:HG2	2.25	0.49
1:C:129:SER:HB3	1:D:132:TYR:HD1	1.76	0.49
1:A:169:GLU:HB2	1:A:247:HIS:HE1	1.77	0.49
1:G:122:LEU:O	1:G:123:GLY:C	2.41	0.49
1:F:54:THR:O	1:F:57:TYR:HB3	2.13	0.49
1:B:54:THR:O	1:B:57:TYR:HB3	2.13	0.49
1:G:219:ASP:C	1:G:219:ASP:OD1	2.49	0.49
1:D:219:ASP:C	1:D:219:ASP:OD1	2.49	0.49
1:F:116:GLU:O	1:F:119:CYS:N	2.45	0.49
1:A:280:ASP:O	1:A:280:ASP:OD1	2.30	0.49
1:F:280:ASP:O	1:F:280:ASP:OD1	2.30	0.49
1:E:61:ASN:ND2	1:E:94:MET:HE2	2.26	0.49
1:C:61:ASN:OD1	1:C:94:MET:HE2	2.12	0.49
1:E:44:VAL:CG1	1:E:45:SER:N	2.75	0.49
1:C:200:LEU:HD13	1:C:214:VAL:HG12	1.93	0.49
1:C:162:ARG:O	1:C:290:PHE:HZ	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:PHE:O	1:F:154:GLU:C	2.50	0.49
1:G:76:GLU:HG3	1:G:77:ASN:ND2	2.28	0.49
1:E:169:GLU:HB2	1:E:247:HIS:HE1	1.77	0.49
1:C:116:GLU:O	1:C:119:CYS:N	2.45	0.49
1:B:172:ILE:O	1:B:173:GLU:CG	2.61	0.49
1:A:88:PHE:CE2	1:D:110:ASN:HB3	2.47	0.49
1:H:204:ARG:CG	1:H:204:ARG:HH11	2.23	0.49
1:H:49:PHE:HE2	1:H:131:ILE:HD13	1.77	0.49
1:C:104:PRO:CB	1:C:110:ASN:OD1	2.61	0.49
1:C:141:GLY:O	1:C:166:LEU:HB2	2.12	0.49
1:C:169:GLU:HB2	1:C:247:HIS:HE1	1.77	0.49
1:B:76:GLU:HG3	1:B:77:ASN:ND2	2.28	0.49
1:G:104:PRO:CG	1:G:110:ASN:OD1	2.61	0.49
1:D:172:ILE:O	1:D:173:GLU:CG	2.61	0.49
1:H:201:THR:HG23	1:H:217:PRO:HD3	1.93	0.49
1:B:44:VAL:CG1	1:B:45:SER:N	2.75	0.49
1:E:154:GLU:CA	1:H:188:GLU:OE2	2.60	0.49
1:A:200:LEU:HD13	1:A:214:VAL:HG12	1.92	0.49
1:G:54:THR:O	1:G:57:TYR:HB3	2.13	0.49
1:H:172:ILE:O	1:H:173:GLU:CG	2.61	0.49
1:C:185:ILE:HD11	1:C:191:VAL:HB	1.92	0.49
1:D:200:LEU:HD13	1:D:214:VAL:HG12	1.92	0.49
1:A:145:SER:O	1:A:260:TYR:OH	2.24	0.49
1:E:54:THR:O	1:E:57:TYR:HB3	2.13	0.49
1:G:182:ARG:CB	1:G:237:SER:HB3	2.43	0.49
1:A:172:ILE:O	1:A:173:GLU:CG	2.61	0.49
1:E:172:ILE:O	1:E:173:GLU:CG	2.61	0.49
1:F:44:VAL:CG1	1:F:45:SER:N	2.75	0.49
1:H:200:LEU:HD13	1:H:214:VAL:HG12	1.92	0.49
1:A:153:PHE:CE2	1:A:154:GLU:HB2	2.48	0.49
1:C:295:GLN:O	1:E:292:GLU:HA	2.12	0.49
1:A:141:GLY:O	1:A:166:LEU:N	2.43	0.49
1:C:74:VAL:HB	1:C:109:ALA:HB2	1.95	0.49
1:E:116:GLU:O	1:E:119:CYS:N	2.45	0.48
1:D:266:ILE:CD1	1:D:293:ILE:HD12	2.39	0.48
1:H:266:ILE:CD1	1:H:293:ILE:HD12	2.42	0.48
1:D:110:ASN:O	1:D:113:VAL:HB	2.12	0.48
1:E:153:PHE:CD2	1:E:154:GLU:HB2	2.48	0.48
1:D:185:ILE:HD11	1:D:191:VAL:HB	1.92	0.48
1:D:46:TRP:N	1:D:47:PRO:HD2	2.28	0.48
1:H:192:PHE:HE1	1:H:194:ARG:HB2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:LEU:O	1:G:72:GLY:N	2.45	0.48
1:E:280:ASP:CB	1:E:282:ARG:HG2	2.39	0.48
1:E:23:ILE:HG13	1:F:283:ARG:HH21	1.78	0.48
1:H:169:GLU:HB2	1:H:247:HIS:HE1	1.77	0.48
1:C:182:ARG:HA	1:C:193:ARG:NH1	2.28	0.48
1:C:153:PHE:CE2	1:C:154:GLU:HB2	2.48	0.48
1:D:153:PHE:O	1:D:154:GLU:C	2.51	0.48
1:D:153:PHE:CE2	1:D:154:GLU:HB2	2.48	0.48
1:F:153:PHE:CE2	1:F:154:GLU:HB2	2.48	0.48
1:G:182:ARG:HB3	1:G:237:SER:HB3	1.95	0.48
1:G:204:ARG:NH1	1:G:204:ARG:HG2	2.25	0.48
1:H:75:ILE:CD1	1:H:89:PHE:HD2	2.21	0.48
1:A:201:THR:HG23	1:A:217:PRO:HD3	1.93	0.48
1:D:149:VAL:HG12	1:D:293:ILE:HD13	1.96	0.48
1:E:153:PHE:CE2	1:E:154:GLU:HB2	2.48	0.48
1:C:153:PHE:O	1:C:154:GLU:C	2.51	0.48
1:H:153:PHE:CE2	1:H:154:GLU:HB2	2.48	0.48
1:H:184:GLU:OE1	1:H:194:ARG:HD2	2.13	0.48
1:B:280:ASP:CB	1:B:282:ARG:HG2	2.39	0.48
1:E:61:ASN:OD1	1:E:94:MET:HE2	2.13	0.48
1:C:153:PHE:CD2	1:C:154:GLU:HB2	2.48	0.48
1:A:153:PHE:CD2	1:A:154:GLU:HB2	2.48	0.48
1:B:46:TRP:N	1:B:47:PRO:HD2	2.28	0.48
1:G:172:ILE:O	1:G:173:GLU:CG	2.61	0.48
1:F:172:ILE:O	1:F:173:GLU:CG	2.62	0.48
1:G:201:THR:CG2	1:G:217:PRO:CD	2.90	0.48
1:E:44:VAL:CG1	1:E:48:VAL:CB	2.91	0.48
1:H:110:ASN:O	1:H:113:VAL:HB	2.12	0.48
1:B:153:PHE:CE2	1:B:154:GLU:HB2	2.48	0.48
1:H:153:PHE:CD2	1:H:154:GLU:HB2	2.48	0.48
1:A:46:TRP:N	1:A:47:PRO:HD2	2.28	0.48
1:F:46:TRP:N	1:F:47:PRO:HD2	2.28	0.48
1:F:76:GLU:HG3	1:F:77:ASN:ND2	2.28	0.48
1:D:68:TYR:O	1:D:69:LEU:C	2.52	0.48
1:E:26:LEU:N	1:F:285:ILE:O	2.46	0.48
1:A:23:ILE:HG21	1:B:285:ILE:HG13	1.96	0.48
1:H:93:THR:CG2	1:H:116:GLU:OE1	2.60	0.48
1:G:14:ILE:CG2	1:H:283:ARG:NH1	2.77	0.48
1:D:204:ARG:NH1	1:D:204:ARG:HG2	2.25	0.48
1:H:44:VAL:HG13	1:H:48:VAL:HB	1.94	0.48
1:D:153:PHE:CD2	1:D:154:GLU:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:TRP:N	1:H:47:PRO:HD2	2.28	0.48
1:E:75:ILE:O	1:E:76:GLU:C	2.50	0.48
1:D:201:THR:CG2	1:D:217:PRO:CD	2.90	0.48
1:F:201:THR:CG2	1:F:217:PRO:CD	2.90	0.48
1:C:44:VAL:HG11	1:C:48:VAL:HG12	1.96	0.48
1:H:153:PHE:O	1:H:154:GLU:C	2.51	0.48
1:B:68:TYR:O	1:B:69:LEU:C	2.52	0.48
1:A:266:ILE:CD1	1:A:293:ILE:HD12	2.40	0.48
1:A:162:ARG:O	1:A:290:PHE:HZ	1.96	0.48
1:F:116:GLU:O	1:F:119:CYS:HB2	2.14	0.47
1:F:172:ILE:O	1:F:173:GLU:C	2.47	0.47
1:C:185:ILE:HD11	1:C:191:VAL:CG2	2.44	0.47
1:F:153:PHE:CD2	1:F:154:GLU:HB2	2.48	0.47
1:D:64:PHE:O	1:D:67:ALA:HB3	2.14	0.47
1:A:116:GLU:O	1:A:119:CYS:HB2	2.14	0.47
1:B:116:GLU:O	1:B:119:CYS:HB2	2.14	0.47
1:D:185:ILE:HD11	1:D:191:VAL:CG2	2.44	0.47
1:G:185:ILE:HD11	1:G:191:VAL:HB	1.92	0.47
1:G:121:MET:O	1:G:124:LEU:N	2.47	0.47
1:E:201:THR:HG23	1:E:217:PRO:HD3	1.93	0.47
1:C:201:THR:CG2	1:C:217:PRO:CD	2.90	0.47
1:F:185:ILE:HD11	1:F:191:VAL:CG2	2.44	0.47
1:G:185:ILE:HD11	1:G:191:VAL:CG2	2.45	0.47
1:A:130:LEU:HD21	1:B:135:PHE:HE2	1.79	0.47
1:B:153:PHE:CD2	1:B:154:GLU:HB2	2.48	0.47
1:G:153:PHE:CD2	1:G:154:GLU:HB2	2.48	0.47
1:G:153:PHE:CE2	1:G:154:GLU:HB2	2.48	0.47
1:G:68:TYR:O	1:G:69:LEU:C	2.52	0.47
1:H:64:PHE:O	1:H:67:ALA:HB3	2.14	0.47
1:G:145:SER:O	1:G:260:TYR:OH	2.24	0.47
1:D:116:GLU:O	1:D:119:CYS:HB2	2.14	0.47
1:E:116:GLU:O	1:E:119:CYS:HB2	2.14	0.47
1:G:210:LEU:CD1	1:G:285:ILE:HD11	2.34	0.47
1:F:243:PHE:CD2	1:F:243:PHE:C	2.88	0.47
1:A:89:PHE:HB2	1:A:102:LEU:HD13	1.96	0.47
1:F:266:ILE:CD1	1:F:293:ILE:HD12	2.42	0.47
1:G:266:ILE:CD1	1:G:293:ILE:HD12	2.42	0.47
1:D:106:GLY:O	1:D:110:ASN:ND2	2.48	0.47
1:C:46:TRP:N	1:C:47:PRO:HD2	2.28	0.47
1:B:16:ASN:O	1:B:259:ALA:HB3	2.15	0.47
1:A:57:TYR:HE1	1:A:94:MET:HE3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:GLU:O	1:G:119:CYS:HB2	2.14	0.47
1:F:64:PHE:O	1:F:67:ALA:HB3	2.14	0.47
1:B:56:LEU:HD12	1:B:60:THR:CG2	2.45	0.47
1:C:266:ILE:CD1	1:C:293:ILE:HD12	2.42	0.47
1:G:64:PHE:O	1:G:67:ALA:HB3	2.14	0.47
1:E:124:LEU:CD1	1:H:121:MET:HB3	2.45	0.47
1:B:185:ILE:HD11	1:B:191:VAL:CG2	2.44	0.47
1:A:185:ILE:HD11	1:A:191:VAL:CG2	2.44	0.47
1:H:185:ILE:HD11	1:H:191:VAL:CG2	2.44	0.47
1:B:175:ASP:OD2	1:B:204:ARG:NH1	2.48	0.47
1:A:153:PHE:O	1:A:154:GLU:C	2.51	0.47
1:C:243:PHE:CD2	1:C:243:PHE:C	2.88	0.47
1:A:42:LEU:HB3	1:A:137:ARG:NH2	2.30	0.47
1:F:61:ASN:ND2	1:F:94:MET:HE2	2.29	0.47
1:C:116:GLU:O	1:C:119:CYS:HB2	2.14	0.47
1:H:56:LEU:HD12	1:H:60:THR:CG2	2.45	0.47
1:G:23:ILE:CG2	1:H:285:ILE:HG13	2.40	0.47
1:E:153:PHE:O	1:E:154:GLU:C	2.51	0.47
1:E:166:LEU:HA	1:E:166:LEU:HD23	1.73	0.47
1:B:64:PHE:O	1:B:67:ALA:HB3	2.14	0.47
1:F:56:LEU:HD12	1:F:60:THR:CG2	2.45	0.47
1:H:42:LEU:HB3	1:H:137:ARG:NH2	2.30	0.47
1:E:272:VAL:CG1	1:E:273:ASP:H	2.25	0.47
1:E:185:ILE:HD11	1:E:191:VAL:CG2	2.45	0.47
1:B:204:ARG:HG2	1:B:204:ARG:NH1	2.25	0.47
1:E:175:ASP:OD2	1:E:204:ARG:NH1	2.48	0.47
1:A:49:PHE:CE2	1:A:131:ILE:HD13	2.50	0.47
1:E:68:TYR:O	1:E:69:LEU:C	2.52	0.47
1:A:93:THR:HG21	1:A:116:GLU:OE1	2.15	0.47
1:E:266:ILE:CD1	1:E:293:ILE:HD12	2.41	0.47
1:A:185:ILE:HD11	1:A:191:VAL:HB	1.92	0.47
1:A:124:LEU:CD1	1:D:121:MET:HB3	2.45	0.47
1:G:175:ASP:OD2	1:G:204:ARG:NH1	2.48	0.46
1:E:23:ILE:HD11	1:F:283:ARG:CZ	2.45	0.46
1:H:116:GLU:O	1:H:119:CYS:HB2	2.14	0.46
1:D:175:ASP:OD2	1:D:204:ARG:NH1	2.48	0.46
1:H:243:PHE:CD2	1:H:243:PHE:C	2.88	0.46
1:B:151:SER:HB3	1:B:269:GLY:O	2.15	0.46
1:E:244:THR:HG22	1:E:255:HIS:HB2	1.97	0.46
1:H:175:ASP:OD2	1:H:204:ARG:NH1	2.48	0.46
1:F:280:ASP:CB	1:F:282:ARG:HG2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:ILE:HD11	1:H:89:PHE:CD2	2.46	0.46
1:C:56:LEU:HD12	1:C:60:THR:CG2	2.45	0.46
1:B:201:THR:HG23	1:B:217:PRO:HD3	1.93	0.46
1:A:92:GLN:OE1	1:A:99:TYR:HD1	1.97	0.46
1:C:175:ASP:OD2	1:C:204:ARG:NH1	2.48	0.46
1:A:175:ASP:OD2	1:A:204:ARG:NH1	2.48	0.46
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.73	0.46
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.72	0.46
1:A:284:ALA:HA	1:D:23:ILE:CG2	2.45	0.46
1:G:104:PRO:HB2	1:G:110:ASN:OD1	2.15	0.46
1:E:56:LEU:HD12	1:E:60:THR:CG2	2.45	0.46
1:D:201:THR:HG23	1:D:217:PRO:HD3	1.93	0.46
1:A:147:ARG:HB2	1:A:293:ILE:HD11	1.97	0.46
1:B:266:ILE:CD1	1:B:293:ILE:HD12	2.42	0.46
1:H:272:VAL:CG1	1:H:273:ASP:H	2.25	0.46
1:E:147:ARG:HH11	1:E:147:ARG:HG2	1.81	0.46
1:B:147:ARG:HG2	1:B:147:ARG:HH11	1.81	0.46
1:G:56:LEU:HD12	1:G:60:THR:CG2	2.45	0.46
1:G:243:PHE:C	1:G:243:PHE:CD2	2.88	0.46
1:C:64:PHE:O	1:C:67:ALA:HB3	2.14	0.46
1:A:243:PHE:C	1:A:243:PHE:CD2	2.88	0.46
1:E:243:PHE:CD2	1:E:243:PHE:C	2.88	0.46
1:H:121:MET:C	1:H:123:GLY:N	2.68	0.46
1:A:272:VAL:CG1	1:A:273:ASP:H	2.25	0.46
1:E:130:LEU:O	1:E:131:ILE:C	2.54	0.46
1:H:104:PRO:CG	1:H:110:ASN:OD1	2.63	0.46
1:B:244:THR:HG22	1:B:255:HIS:HB2	1.97	0.46
1:A:64:PHE:O	1:A:67:ALA:HB3	2.14	0.46
1:E:18:ASP:O	1:E:257:ARG:NH1	2.49	0.46
1:A:94:MET:C	1:A:95:ALA:C	2.69	0.46
1:A:266:ILE:HG22	1:A:269:GLY:HA3	1.98	0.46
1:B:204:ARG:CG	1:B:204:ARG:NH1	2.79	0.46
1:H:130:LEU:O	1:H:131:ILE:C	2.54	0.46
1:C:114:THR:HG22	1:D:91:VAL:HG21	1.98	0.46
1:B:243:PHE:C	1:B:243:PHE:CD2	2.88	0.46
1:C:147:ARG:HH11	1:C:147:ARG:HG2	1.81	0.46
1:C:201:THR:HG23	1:C:217:PRO:HD3	1.93	0.46
1:E:154:GLU:H	1:H:188:GLU:CD	2.19	0.46
1:H:147:ARG:HH11	1:H:147:ARG:HG2	1.81	0.46
1:E:64:PHE:O	1:E:67:ALA:HB3	2.14	0.46
1:F:244:THR:HG22	1:F:255:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:LEU:HB3	1:F:285:ILE:CD1	2.45	0.46
1:F:114:THR:CG2	1:G:91:VAL:HG21	2.46	0.46
1:F:130:LEU:HD21	1:G:135:PHE:HE2	1.81	0.46
1:G:166:LEU:HD23	1:G:166:LEU:HA	1.73	0.46
1:B:141:GLY:O	1:B:166:LEU:CB	2.64	0.46
1:E:181:VAL:HG12	1:E:193:ARG:CZ	2.44	0.46
1:F:69:LEU:HD23	1:F:69:LEU:HA	1.66	0.46
1:C:244:THR:HG22	1:C:255:HIS:HB2	1.97	0.46
1:G:92:GLN:OE1	1:G:99:TYR:HD1	1.99	0.46
1:A:56:LEU:HD12	1:A:60:THR:CG2	2.45	0.46
1:D:56:LEU:HD12	1:D:60:THR:CG2	2.45	0.46
1:G:244:THR:HG22	1:G:255:HIS:HB2	1.97	0.46
1:A:244:THR:HG22	1:A:255:HIS:HB2	1.98	0.46
1:G:89:PHE:HD1	1:G:102:LEU:HB2	1.78	0.45
1:G:114:THR:CG2	1:H:88:PHE:CE2	2.99	0.45
1:A:204:ARG:NH1	1:A:204:ARG:CG	2.79	0.45
1:H:49:PHE:CE2	1:H:131:ILE:HD13	2.51	0.45
1:B:114:THR:HG22	1:C:91:VAL:HG21	1.97	0.45
1:G:38:TYR:OH	1:H:136:THR:HG22	2.16	0.45
1:D:243:PHE:C	1:D:243:PHE:CD2	2.88	0.45
1:A:201:THR:CG2	1:A:217:PRO:CD	2.90	0.45
1:F:185:ILE:HD13	1:F:191:VAL:HA	1.99	0.45
1:B:104:PRO:CG	1:B:110:ASN:OD1	2.64	0.45
1:H:71:CYS:HB2	1:H:74:VAL:CG2	2.46	0.45
1:F:147:ARG:HH11	1:F:147:ARG:HG2	1.81	0.45
1:B:38:TYR:OH	1:C:136:THR:HG22	2.17	0.45
1:B:75:ILE:HD11	1:B:89:PHE:CE2	2.51	0.45
1:B:272:VAL:CG1	1:B:273:ASP:H	2.25	0.45
1:H:68:TYR:O	1:H:69:LEU:C	2.52	0.45
1:C:185:ILE:CD1	1:C:191:VAL:HG23	2.47	0.45
1:E:204:ARG:NH1	1:E:204:ARG:HG2	2.25	0.45
1:G:49:PHE:HE2	1:G:131:ILE:CD1	2.29	0.45
1:A:130:LEU:O	1:A:131:ILE:C	2.54	0.45
1:F:130:LEU:O	1:F:131:ILE:C	2.54	0.45
1:E:181:VAL:HG12	1:E:193:ARG:NH2	2.31	0.45
1:C:68:TYR:O	1:C:69:LEU:C	2.52	0.45
1:H:94:MET:HB2	1:H:116:GLU:CG	2.45	0.45
1:G:185:ILE:CD1	1:G:191:VAL:HG23	2.47	0.45
1:H:204:ARG:NH1	1:H:204:ARG:CG	2.79	0.45
1:H:141:GLY:O	1:H:166:LEU:CB	2.64	0.45
1:E:88:PHE:CE2	1:H:110:ASN:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:ALA:O	1:E:96:THR:OG1	2.34	0.45
1:F:104:PRO:CG	1:F:110:ASN:OD1	2.64	0.45
1:E:154:GLU:N	1:H:188:GLU:CD	2.69	0.45
1:D:244:THR:HG22	1:D:255:HIS:HB2	1.97	0.45
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.81	0.45
1:D:185:ILE:CD1	1:D:191:VAL:HG23	2.47	0.45
1:C:44:VAL:HG11	1:C:48:VAL:CG1	2.46	0.45
1:F:15:LEU:HB2	1:F:238:GLU:OE1	2.16	0.45
1:A:68:TYR:O	1:A:69:LEU:C	2.52	0.45
1:A:143:LEU:O	1:A:163:LEU:HA	2.17	0.45
1:A:278:LEU:HG	1:A:282:ARG:O	2.17	0.45
1:D:61:ASN:ND2	1:D:94:MET:HE2	2.31	0.45
1:B:117:ALA:O	1:B:118:LEU:C	2.55	0.45
1:F:185:ILE:CD1	1:F:191:VAL:HG23	2.47	0.45
1:E:185:ILE:CD1	1:E:191:VAL:HG23	2.47	0.45
1:F:41:LEU:O	1:F:134:ARG:NH1	2.49	0.45
1:D:141:GLY:O	1:D:166:LEU:CB	2.64	0.45
1:G:141:GLY:O	1:G:166:LEU:CB	2.64	0.45
1:E:75:ILE:C	1:E:76:GLU:O	2.48	0.45
1:C:75:ILE:CD1	1:C:89:PHE:CE2	2.99	0.45
1:F:201:THR:HG23	1:F:217:PRO:HD3	1.92	0.45
1:B:185:ILE:CD1	1:B:191:VAL:HG23	2.47	0.45
1:D:204:ARG:CG	1:D:204:ARG:NH1	2.79	0.45
1:D:130:LEU:O	1:D:131:ILE:C	2.54	0.45
1:G:130:LEU:O	1:G:131:ILE:C	2.54	0.45
1:F:68:TYR:O	1:F:69:LEU:C	2.52	0.45
1:A:284:ALA:HA	1:D:23:ILE:HG22	1.99	0.45
1:G:278:LEU:HG	1:G:282:ARG:O	2.17	0.45
1:E:173:GLU:N	1:E:206:PRO:O	2.44	0.45
1:A:185:ILE:CD1	1:A:191:VAL:HG23	2.47	0.45
1:E:185:ILE:HD13	1:E:191:VAL:HA	1.99	0.45
1:B:130:LEU:O	1:B:131:ILE:C	2.54	0.45
1:H:44:VAL:HG12	1:H:45:SER:O	2.17	0.45
1:E:114:THR:HG22	1:F:91:VAL:HG21	1.99	0.44
1:D:278:LEU:HG	1:D:282:ARG:O	2.17	0.44
1:D:117:ALA:O	1:D:120:GLY:N	2.50	0.44
1:C:117:ALA:O	1:C:120:GLY:N	2.50	0.44
1:F:174:ALA:HB1	1:F:243:PHE:CE1	2.52	0.44
1:D:147:ARG:HG2	1:D:147:ARG:HH11	1.81	0.44
1:G:185:ILE:HD13	1:G:191:VAL:HA	1.99	0.44
1:C:110:ASN:HB3	1:D:88:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HG22	1:D:38:TYR:OH	2.17	0.44
1:A:93:THR:O	1:A:96:THR:N	2.46	0.44
1:G:204:ARG:NH1	1:G:204:ARG:CG	2.79	0.44
1:H:89:PHE:HB2	1:H:102:LEU:HD13	1.98	0.44
1:F:110:ASN:HB2	1:G:88:PHE:CZ	2.52	0.44
1:C:93:THR:CG2	1:C:116:GLU:OE1	2.65	0.44
1:C:61:ASN:ND2	1:C:94:MET:HE2	2.30	0.44
1:C:185:ILE:HD13	1:C:191:VAL:HA	1.99	0.44
1:A:273:ASP:OD1	1:A:274:VAL:N	2.50	0.44
1:F:204:ARG:HH11	1:F:204:ARG:CG	2.24	0.44
1:E:41:LEU:O	1:E:134:ARG:NH1	2.50	0.44
1:F:46:TRP:O	1:F:50:ILE:HG13	2.17	0.44
1:F:117:ALA:O	1:F:120:GLY:N	2.50	0.44
1:B:278:LEU:HG	1:B:282:ARG:O	2.17	0.44
1:E:278:LEU:HB3	1:E:279:PRO:HD2	1.99	0.44
1:G:242:LEU:HD12	1:G:243:PHE:N	2.33	0.44
1:H:117:ALA:O	1:H:118:LEU:C	2.55	0.44
1:G:272:VAL:CG1	1:G:273:ASP:H	2.25	0.44
1:C:130:LEU:O	1:C:131:ILE:C	2.54	0.44
1:C:192:PHE:HE1	1:C:194:ARG:HB2	1.82	0.44
1:G:147:ARG:HG2	1:G:147:ARG:HH11	1.81	0.44
1:H:242:LEU:HD12	1:H:243:PHE:N	2.33	0.44
1:D:242:LEU:HD12	1:D:243:PHE:N	2.33	0.44
1:A:283:ARG:HB3	1:D:23:ILE:CD1	2.47	0.44
1:H:278:LEU:HB3	1:H:279:PRO:HD2	2.00	0.44
1:H:278:LEU:HG	1:H:282:ARG:O	2.17	0.44
1:B:278:LEU:HB3	1:B:279:PRO:HD2	2.00	0.44
1:E:124:LEU:HD11	1:H:121:MET:HB3	1.99	0.44
1:A:185:ILE:HD13	1:A:191:VAL:HA	1.99	0.44
1:E:49:PHE:HE2	1:E:131:ILE:CD1	2.28	0.44
1:A:242:LEU:HD12	1:A:243:PHE:N	2.33	0.44
1:C:42:LEU:HB3	1:C:137:ARG:NH2	2.33	0.44
1:C:278:LEU:HG	1:C:282:ARG:O	2.17	0.44
1:F:278:LEU:HG	1:F:282:ARG:O	2.17	0.44
1:E:278:LEU:HG	1:E:282:ARG:O	2.17	0.44
1:C:75:ILE:HD11	1:C:89:PHE:CE2	2.51	0.44
1:G:110:ASN:CB	1:H:88:PHE:CE2	3.00	0.44
1:E:154:GLU:HA	1:H:188:GLU:OE2	2.17	0.44
1:D:185:ILE:HD13	1:D:191:VAL:HA	1.99	0.44
1:H:185:ILE:HD13	1:H:191:VAL:HA	1.99	0.44
1:C:278:LEU:HB3	1:C:279:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:THR:CG2	1:D:116:GLU:CD	2.86	0.44
1:B:185:ILE:HD13	1:B:191:VAL:HA	1.99	0.44
1:C:147:ARG:HH22	1:E:299:HIS:HA	1.82	0.44
1:A:117:ALA:O	1:A:120:GLY:N	2.50	0.44
1:D:166:LEU:HA	1:D:166:LEU:HD23	1.73	0.44
1:B:242:LEU:HD12	1:B:243:PHE:N	2.33	0.44
1:E:242:LEU:HD12	1:E:243:PHE:N	2.33	0.44
1:D:210:LEU:HD22	1:D:285:ILE:HD12	1.98	0.44
1:H:185:ILE:CD1	1:H:191:VAL:HG23	2.47	0.44
1:C:104:PRO:CG	1:C:110:ASN:OD1	2.66	0.44
1:D:278:LEU:HB3	1:D:279:PRO:HD2	2.00	0.44
1:E:24:THR:O	1:F:285:ILE:N	2.36	0.44
1:E:117:ALA:O	1:E:118:LEU:C	2.55	0.44
1:B:173:GLU:N	1:B:206:PRO:O	2.44	0.44
1:H:210:LEU:HD13	1:H:285:ILE:HD11	2.00	0.44
1:E:135:PHE:HE2	1:H:130:LEU:HD21	1.82	0.44
1:A:239:PHE:CE1	1:A:265:ILE:HD11	2.53	0.44
1:C:280:ASP:CB	1:C:282:ARG:HG2	2.39	0.43
1:A:278:LEU:HB3	1:A:279:PRO:HD2	1.99	0.43
1:F:278:LEU:HB3	1:F:279:PRO:HD2	1.99	0.43
1:G:278:LEU:HB3	1:G:279:PRO:HD2	2.00	0.43
1:H:92:GLN:NE2	1:H:99:TYR:HD1	2.16	0.43
1:F:114:THR:CG2	1:G:88:PHE:CD2	3.00	0.43
1:H:117:ALA:O	1:H:120:GLY:N	2.50	0.43
1:H:239:PHE:CE1	1:H:265:ILE:HD11	2.53	0.43
1:E:182:ARG:CB	1:E:237:SER:HB3	2.48	0.43
1:G:61:ASN:ND2	1:G:94:MET:HE2	2.30	0.43
1:G:26:LEU:HB2	1:H:285:ILE:O	2.18	0.43
1:A:240:LEU:HD21	1:B:207:ILE:CD1	2.48	0.43
1:B:69:LEU:HA	1:B:69:LEU:HD23	1.67	0.43
1:B:239:PHE:CE1	1:B:265:ILE:HD11	2.54	0.43
1:B:117:ALA:O	1:B:120:GLY:N	2.50	0.43
1:H:201:THR:CG2	1:H:217:PRO:CD	2.90	0.43
1:C:49:PHE:CZ	1:C:53:ILE:HD11	2.54	0.43
1:E:49:PHE:CZ	1:E:53:ILE:HD11	2.54	0.43
1:E:239:PHE:CE1	1:E:265:ILE:HD11	2.54	0.43
1:G:114:THR:HG21	1:H:88:PHE:CE2	2.54	0.43
1:F:242:LEU:HD12	1:F:243:PHE:N	2.33	0.43
1:F:242:LEU:HD23	1:G:206:PRO:HB3	1.99	0.43
1:A:39:HIS:HA	1:B:250:PHE:HE2	1.82	0.43
1:D:49:PHE:CZ	1:D:53:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:CZ	1:A:53:ILE:HD11	2.54	0.43
1:C:242:LEU:HD12	1:C:243:PHE:N	2.33	0.43
1:A:117:ALA:O	1:A:118:LEU:C	2.55	0.43
1:G:280:ASP:CB	1:G:282:ARG:HG2	2.39	0.43
1:E:154:GLU:N	1:H:188:GLU:OE2	2.51	0.43
1:G:49:PHE:CZ	1:G:53:ILE:HD11	2.54	0.43
1:B:49:PHE:CZ	1:B:53:ILE:HD11	2.54	0.43
1:E:46:TRP:O	1:E:47:PRO:C	2.56	0.43
1:F:239:PHE:CE1	1:F:265:ILE:HD11	2.53	0.43
1:F:210:LEU:HB3	1:F:285:ILE:HD13	1.99	0.43
1:G:46:TRP:N	1:G:47:PRO:CD	2.78	0.43
1:H:103:ILE:CG2	1:H:104:PRO:HD2	2.49	0.43
1:C:239:PHE:CE1	1:C:265:ILE:HD11	2.54	0.43
1:H:75:ILE:CG2	1:H:102:LEU:HB3	2.49	0.43
1:G:117:ALA:O	1:G:120:GLY:N	2.51	0.43
1:B:191:VAL:HG13	1:B:191:VAL:O	2.19	0.43
1:E:204:ARG:CG	1:E:204:ARG:NH1	2.79	0.43
1:H:49:PHE:CZ	1:H:53:ILE:HD11	2.54	0.43
1:B:110:ASN:HB3	1:C:88:PHE:CD2	2.54	0.43
1:E:129:SER:HB3	1:F:132:TYR:CD1	2.53	0.43
1:G:239:PHE:CE1	1:G:265:ILE:HD11	2.53	0.43
1:D:239:PHE:CE1	1:D:265:ILE:HD11	2.54	0.43
1:E:117:ALA:O	1:E:120:GLY:N	2.51	0.43
1:E:103:ILE:CG2	1:E:104:PRO:HD2	2.49	0.43
1:F:49:PHE:CZ	1:F:53:ILE:HD11	2.54	0.43
1:A:210:LEU:HB3	1:A:285:ILE:HD13	2.01	0.43
1:B:75:ILE:CG2	1:B:102:LEU:HB3	2.49	0.43
1:G:103:ILE:CG2	1:G:104:PRO:HD2	2.49	0.43
1:G:44:VAL:CG1	1:G:48:VAL:CG1	2.97	0.43
1:D:49:PHE:HE2	1:D:131:ILE:HD13	1.84	0.43
1:E:141:GLY:O	1:E:166:LEU:CB	2.64	0.43
1:C:103:ILE:CG2	1:C:104:PRO:HD2	2.49	0.43
1:B:280:ASP:OD2	1:B:282:ARG:CD	2.54	0.43
1:E:75:ILE:CD1	1:E:89:PHE:CE2	2.97	0.43
1:G:94:MET:O	1:G:94:MET:HG2	2.18	0.43
1:D:103:ILE:CG2	1:D:104:PRO:HD2	2.49	0.43
1:B:49:PHE:HE2	1:B:131:ILE:HD13	1.84	0.43
1:B:130:LEU:HD21	1:C:135:PHE:HE2	1.83	0.43
1:H:16:ASN:O	1:H:259:ALA:HB3	2.18	0.43
1:C:18:ASP:O	1:C:257:ARG:NH1	2.51	0.43
1:D:75:ILE:CG2	1:D:102:LEU:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ILE:CG2	1:E:102:LEU:HB3	2.49	0.42
1:F:75:ILE:CG2	1:F:102:LEU:HB3	2.49	0.42
1:D:117:ALA:O	1:D:118:LEU:C	2.56	0.42
1:H:137:ARG:HA	1:H:138:PRO:HD3	1.82	0.42
1:C:49:PHE:HE2	1:C:131:ILE:CD1	2.31	0.42
1:A:103:ILE:CG2	1:A:104:PRO:HD2	2.49	0.42
1:B:129:SER:HB3	1:C:132:TYR:HD1	1.84	0.42
1:E:161:MET:HE3	1:E:161:MET:HB2	1.89	0.42
1:C:75:ILE:CG2	1:C:102:LEU:HB3	2.49	0.42
1:G:75:ILE:CG2	1:G:102:LEU:HB3	2.49	0.42
1:A:75:ILE:CG2	1:A:102:LEU:HB3	2.49	0.42
1:F:39:HIS:HA	1:G:250:PHE:HE2	1.84	0.42
1:G:44:VAL:HG12	1:G:45:SER:N	2.34	0.42
1:D:191:VAL:O	1:D:191:VAL:HG13	2.19	0.42
1:A:145:SER:OG	1:A:161:MET:HB2	2.19	0.42
1:A:166:LEU:HA	1:A:166:LEU:HD23	1.73	0.42
1:C:24:THR:O	1:D:284:ALA:HA	2.19	0.42
1:B:61:ASN:ND2	1:B:94:MET:HE2	2.26	0.42
1:B:94:MET:HG2	1:B:94:MET:O	2.19	0.42
1:G:117:ALA:O	1:G:118:LEU:C	2.55	0.42
1:H:94:MET:HG2	1:H:94:MET:O	2.19	0.42
1:H:69:LEU:C	1:H:72:GLY:H	2.21	0.42
1:E:94:MET:HB2	1:E:116:GLU:CG	2.47	0.42
1:G:94:MET:HB2	1:G:116:GLU:CG	2.48	0.42
1:F:104:PRO:CB	1:F:110:ASN:OD1	2.67	0.42
1:F:44:VAL:HG12	1:F:45:SER:N	2.34	0.42
1:C:191:VAL:O	1:C:191:VAL:HG13	2.19	0.42
1:A:94:MET:HG2	1:A:94:MET:O	2.19	0.42
1:F:61:ASN:OD1	1:F:90:SER:OG	2.30	0.42
1:F:94:MET:O	1:F:94:MET:HG2	2.19	0.42
1:F:191:VAL:O	1:F:191:VAL:HG13	2.19	0.42
1:H:44:VAL:HG11	1:H:48:VAL:CG1	2.50	0.42
1:B:104:PRO:CB	1:B:110:ASN:OD1	2.67	0.42
1:H:41:LEU:O	1:H:134:ARG:NH1	2.51	0.42
1:F:141:GLY:O	1:F:166:LEU:CB	2.64	0.42
1:G:46:TRP:HB2	1:G:47:PRO:HD3	2.02	0.42
1:B:103:ILE:CG2	1:B:104:PRO:HD2	2.49	0.42
1:F:182:ARG:HB2	1:F:235:SER:HB2	2.01	0.42
1:F:117:ALA:O	1:F:118:LEU:C	2.55	0.42
1:C:94:MET:HG2	1:C:94:MET:O	2.18	0.42
1:B:44:VAL:HG12	1:B:45:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:191:VAL:HG13	1:H:191:VAL:O	2.19	0.42
1:A:103:ILE:HG23	1:A:104:PRO:HD2	2.02	0.42
1:C:69:LEU:HA	1:C:69:LEU:HD23	1.66	0.42
1:D:280:ASP:OD2	1:D:282:ARG:CD	2.54	0.42
1:E:75:ILE:HG22	1:E:76:GLU:O	2.20	0.42
1:E:23:ILE:CD1	1:F:283:ARG:CZ	2.98	0.42
1:D:103:ILE:HG23	1:D:104:PRO:HD2	2.02	0.42
1:G:191:VAL:O	1:G:191:VAL:HG13	2.19	0.42
1:F:46:TRP:O	1:F:47:PRO:C	2.59	0.42
1:A:94:MET:C	1:A:96:THR:N	2.74	0.42
1:F:44:VAL:HG12	1:F:45:SER:O	2.20	0.42
1:E:44:VAL:HG12	1:E:45:SER:O	2.20	0.42
1:D:272:VAL:CG1	1:D:273:ASP:H	2.25	0.42
1:C:44:VAL:HG12	1:C:45:SER:O	2.20	0.42
1:E:103:ILE:HG23	1:E:104:PRO:HD2	2.02	0.42
1:C:117:ALA:O	1:C:118:LEU:C	2.55	0.41
1:H:61:ASN:OD1	1:H:90:SER:OG	2.35	0.41
1:A:191:VAL:HG13	1:A:191:VAL:O	2.19	0.41
1:H:166:LEU:HA	1:H:166:LEU:HD23	1.72	0.41
1:A:162:ARG:O	1:A:290:PHE:CZ	2.73	0.41
1:B:46:TRP:O	1:B:47:PRO:C	2.59	0.41
1:C:146:SER:O	1:C:147:ARG:NH1	2.53	0.41
1:F:146:SER:O	1:F:147:ARG:NH1	2.53	0.41
1:F:61:ASN:CG	1:F:94:MET:HE2	2.40	0.41
1:E:94:MET:O	1:E:94:MET:HG2	2.19	0.41
1:F:103:ILE:CG2	1:F:104:PRO:HD2	2.49	0.41
1:B:44:VAL:HG12	1:B:45:SER:O	2.20	0.41
1:E:191:VAL:HG13	1:E:191:VAL:O	2.19	0.41
1:F:204:ARG:NH1	1:F:204:ARG:CG	2.79	0.41
1:B:131:ILE:H	1:B:131:ILE:HG12	1.74	0.41
1:H:103:ILE:HG23	1:H:104:PRO:HD2	2.02	0.41
1:E:129:SER:HB3	1:F:132:TYR:HD1	1.85	0.41
1:D:45:SER:O	1:D:46:TRP:C	2.58	0.41
1:C:46:TRP:O	1:C:47:PRO:C	2.59	0.41
1:E:39:HIS:HA	1:F:250:PHE:HE2	1.84	0.41
1:E:44:VAL:HG12	1:E:45:SER:N	2.34	0.41
1:H:46:TRP:O	1:H:47:PRO:C	2.58	0.41
1:D:15:LEU:HB2	1:D:238:GLU:OE1	2.20	0.41
1:D:94:MET:O	1:D:94:MET:HG2	2.18	0.41
1:B:94:MET:HB2	1:B:116:GLU:CG	2.48	0.41
1:F:111:THR:N	1:G:88:PHE:CE2	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:VAL:HG12	1:G:45:SER:O	2.20	0.41
1:A:44:VAL:HG12	1:A:45:SER:N	2.34	0.41
1:E:88:PHE:CE2	1:H:114:THR:CG2	3.03	0.41
1:C:292:GLU:HG2	1:E:295:GLN:O	2.21	0.41
1:D:210:LEU:HB3	1:D:285:ILE:HD11	1.98	0.41
1:G:75:ILE:CD1	1:G:89:PHE:CE2	3.03	0.41
1:G:93:THR:HG23	1:G:94:MET:N	2.36	0.41
1:C:168:ILE:CD1	1:C:168:ILE:N	2.61	0.41
1:B:129:SER:HB3	1:C:132:TYR:CD1	2.55	0.41
1:B:198:LEU:HD22	1:B:223:PRO:HD2	2.03	0.41
1:D:94:MET:HB2	1:D:116:GLU:CG	2.48	0.41
1:B:93:THR:HG23	1:B:94:MET:N	2.35	0.41
1:D:185:ILE:HD12	1:D:191:VAL:HB	2.02	0.41
1:C:44:VAL:HG12	1:C:45:SER:N	2.34	0.41
1:B:146:SER:O	1:B:147:ARG:NH1	2.53	0.41
1:E:198:LEU:HD22	1:E:223:PRO:HD2	2.03	0.41
1:C:198:LEU:HD22	1:C:223:PRO:HD2	2.03	0.41
1:F:198:LEU:HD22	1:F:223:PRO:HD2	2.03	0.41
1:F:93:THR:HG23	1:F:94:MET:N	2.36	0.41
1:B:44:VAL:HG13	1:B:48:VAL:CB	2.49	0.41
1:A:92:GLN:O	1:A:97:ILE:N	2.54	0.41
1:A:114:THR:CG2	1:B:91:VAL:HG21	2.51	0.41
1:E:146:SER:O	1:E:147:ARG:NH1	2.53	0.41
1:A:168:ILE:N	1:A:168:ILE:CD1	2.61	0.41
1:G:23:ILE:CD1	1:H:283:ARG:HD3	2.50	0.41
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.72	0.41
1:C:103:ILE:HG23	1:C:104:PRO:HD2	2.02	0.41
1:F:129:SER:HB3	1:G:132:TYR:HD1	1.84	0.41
1:B:103:ILE:HG23	1:B:104:PRO:HD2	2.02	0.41
1:A:46:TRP:O	1:A:47:PRO:C	2.59	0.41
1:D:280:ASP:CB	1:D:282:ARG:HG2	2.39	0.41
1:G:103:ILE:HG23	1:G:104:PRO:HD2	2.02	0.41
1:G:93:THR:CG2	1:G:116:GLU:CD	2.89	0.41
1:F:114:THR:CG2	1:G:88:PHE:CE2	3.04	0.41
1:A:44:VAL:CG1	1:A:48:VAL:CG1	2.99	0.41
1:A:44:VAL:HG12	1:A:45:SER:O	2.20	0.41
1:C:181:VAL:HG12	1:C:193:ARG:CZ	2.51	0.41
1:D:198:LEU:HD22	1:D:223:PRO:HD2	2.03	0.41
1:E:13:ARG:H	1:E:13:ARG:HG2	1.74	0.41
1:E:69:LEU:HD23	1:E:69:LEU:HA	1.66	0.41
1:H:91:VAL:CG2	1:H:92:GLN:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:THR:OG1	1:H:99:TYR:OH	2.28	0.40
1:H:93:THR:HG23	1:H:94:MET:N	2.35	0.40
1:A:92:GLN:HA	1:A:97:ILE:HD12	2.03	0.40
1:D:185:ILE:CD1	1:D:191:VAL:CG2	2.99	0.40
1:E:185:ILE:CD1	1:E:191:VAL:CG2	2.99	0.40
1:C:15:LEU:HB2	1:C:238:GLU:OE1	2.21	0.40
1:D:91:VAL:CG2	1:D:92:GLN:N	2.85	0.40
1:A:193:ARG:NH1	1:A:236:HIS:O	2.46	0.40
1:H:74:VAL:HB	1:H:109:ALA:HB2	2.02	0.40
1:E:23:ILE:HG13	1:F:283:ARG:NH2	2.36	0.40
1:D:61:ASN:HD21	1:D:94:MET:HE2	1.80	0.40
1:A:266:ILE:CG2	1:A:269:GLY:HA3	2.52	0.40
1:A:185:ILE:CD1	1:A:191:VAL:CG2	2.99	0.40
1:H:44:VAL:HG12	1:H:45:SER:N	2.36	0.40
1:D:46:TRP:O	1:D:47:PRO:C	2.58	0.40
1:G:69:LEU:HA	1:G:69:LEU:HD23	1.67	0.40
1:C:292:GLU:HG2	1:E:295:GLN:C	2.42	0.40
1:B:52:LEU:HA	1:B:52:LEU:HD23	1.91	0.40
1:A:98:GLY:HA3	1:B:97:ILE:HG22	2.03	0.40
1:H:69:LEU:HD23	1:H:69:LEU:HA	1.66	0.40
1:C:185:ILE:CD1	1:C:191:VAL:CG2	2.99	0.40
1:A:104:PRO:HB2	1:A:110:ASN:CG	2.42	0.40
1:C:110:ASN:CB	1:D:88:PHE:CE2	3.05	0.40
1:C:91:VAL:CG2	1:C:92:GLN:N	2.85	0.40
1:G:146:SER:O	1:G:147:ARG:NH1	2.53	0.40
1:A:198:LEU:HD22	1:A:223:PRO:HD2	2.03	0.40
1:F:103:ILE:HG23	1:F:104:PRO:HD2	2.02	0.40
1:C:204:ARG:NH1	1:C:204:ARG:CG	2.79	0.40
1:A:69:LEU:HA	1:A:69:LEU:HD23	1.67	0.40
1:A:69:LEU:O	1:A:72:GLY:HA2	2.20	0.40
1:E:93:THR:HG22	1:E:94:MET:N	2.37	0.40
1:G:91:VAL:CG2	1:G:92:GLN:N	2.85	0.40
1:F:158:THR:HG23	1:F:217:PRO:N	2.37	0.40
1:B:185:ILE:CD1	1:B:191:VAL:CG2	2.99	0.40
1:H:131:ILE:H	1:H:131:ILE:HG12	1.74	0.40
1:H:105:ILE:H	1:H:109:ALA:CB	2.34	0.40
1:H:198:LEU:HD22	1:H:223:PRO:HD2	2.03	0.40
1:C:270:HIS:O	1:C:294:ALA:N	2.55	0.40
1:D:192:PHE:HE1	1:D:194:ARG:HB2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/301 (93%)	260 (93%)	18 (6%)	1 (0%)	39	80
1	B	279/301 (93%)	260 (93%)	18 (6%)	1 (0%)	39	80
1	C	279/301 (93%)	259 (93%)	18 (6%)	2 (1%)	26	71
1	D	279/301 (93%)	260 (93%)	18 (6%)	1 (0%)	39	80
1	E	279/301 (93%)	257 (92%)	20 (7%)	2 (1%)	26	71
1	F	279/301 (93%)	257 (92%)	20 (7%)	2 (1%)	26	71
1	G	279/301 (93%)	260 (93%)	18 (6%)	1 (0%)	39	80
1	H	279/301 (93%)	258 (92%)	20 (7%)	1 (0%)	39	80
All	All	2232/2408 (93%)	2071 (93%)	150 (7%)	11 (0%)	34	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	287	LEU
1	E	77	ASN
1	A	59	VAL
1	B	59	VAL
1	C	59	VAL
1	C	287	LEU
1	D	59	VAL
1	E	59	VAL
1	F	59	VAL
1	G	59	VAL
1	H	59	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/256 (92%)	218 (93%)	17 (7%)	18	57
1	B	235/256 (92%)	217 (92%)	18 (8%)	16	53
1	C	235/256 (92%)	218 (93%)	17 (7%)	18	57
1	D	236/256 (92%)	218 (92%)	18 (8%)	16	54
1	E	236/256 (92%)	219 (93%)	17 (7%)	18	57
1	F	236/256 (92%)	218 (92%)	18 (8%)	16	54
1	G	235/256 (92%)	217 (92%)	18 (8%)	16	53
1	H	236/256 (92%)	216 (92%)	20 (8%)	13	49
All	All	1884/2048 (92%)	1741 (92%)	143 (8%)	16	54

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	82	SER
1	A	92	GLN
1	A	93	THR
1	A	114	THR
1	A	129	SER
1	A	134	ARG
1	A	154	GLU
1	A	160	MET
1	A	161	MET
1	A	168	ILE
1	A	170	GLN
1	A	204	ARG
1	A	220	HIS
1	A	235	SER
1	A	262	CYS
1	A	264	GLU
1	B	74	VAL
1	B	82	SER
1	B	92	GLN
1	B	93	THR
1	B	114	THR
1	B	129	SER
1	B	134	ARG

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Mol	Chain	Res	Type
1	B	154	GLU
1	B	160	MET
1	B	161	MET
1	B	168	ILE
1	B	170	GLN
1	B	197	ASP
1	B	204	ARG
1	B	220	HIS
1	B	235	SER
1	B	262	CYS
1	B	264	GLU
1	C	74	VAL
1	C	82	SER
1	C	92	GLN
1	C	93	THR
1	C	114	THR
1	C	129	SER
1	C	134	ARG
1	C	154	GLU
1	C	160	MET
1	C	161	MET
1	C	168	ILE
1	C	170	GLN
1	C	204	ARG
1	C	220	HIS
1	C	235	SER
1	C	262	CYS
1	C	264	GLU
1	D	74	VAL
1	D	82	SER
1	D	92	GLN
1	D	93	THR
1	D	114	THR
1	D	121	MET
1	D	129	SER
1	D	134	ARG
1	D	154	GLU
1	D	160	MET
1	D	161	MET
1	D	168	ILE
1	D	170	GLN
1	D	204	ARG

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Mol	Chain	Res	Type
1	D	220	HIS
1	D	235	SER
1	D	262	CYS
1	D	264	GLU
1	E	74	VAL
1	E	82	SER
1	E	92	GLN
1	E	93	THR
1	E	114	THR
1	E	129	SER
1	E	134	ARG
1	E	154	GLU
1	E	160	MET
1	E	161	MET
1	E	168	ILE
1	E	170	GLN
1	E	204	ARG
1	E	220	HIS
1	E	235	SER
1	E	262	CYS
1	E	264	GLU
1	F	74	VAL
1	F	82	SER
1	F	92	GLN
1	F	93	THR
1	F	114	THR
1	F	129	SER
1	F	134	ARG
1	F	154	GLU
1	F	160	MET
1	F	161	MET
1	F	168	ILE
1	F	170	GLN
1	F	197	ASP
1	F	204	ARG
1	F	220	HIS
1	F	235	SER
1	F	262	CYS
1	F	264	GLU
1	G	74	VAL
1	G	82	SER
1	G	92	GLN

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Mol	Chain	Res	Type
1	G	93	THR
1	G	114	THR
1	G	129	SER
1	G	134	ARG
1	G	154	GLU
1	G	160	MET
1	G	161	MET
1	G	168	ILE
1	G	170	GLN
1	G	197	ASP
1	G	204	ARG
1	G	220	HIS
1	G	235	SER
1	G	262	CYS
1	G	264	GLU
1	H	74	VAL
1	H	82	SER
1	H	92	GLN
1	H	93	THR
1	H	114	THR
1	H	121	MET
1	H	129	SER
1	H	134	ARG
1	H	154	GLU
1	H	156	LYS
1	H	160	MET
1	H	161	MET
1	H	168	ILE
1	H	170	GLN
1	H	204	ARG
1	H	220	HIS
1	H	235	SER
1	H	262	CYS
1	H	264	GLU
1	H	283	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	77	ASN
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	196	HIS
1	A	258	HIS
1	B	61	ASN
1	B	77	ASN
1	B	170	GLN
1	B	258	HIS
1	C	61	ASN
1	C	77	ASN
1	C	196	HIS
1	C	258	HIS
1	D	61	ASN
1	D	77	ASN
1	D	258	HIS
1	E	61	ASN
1	E	170	GLN
1	E	246	HIS
1	E	253	ASN
1	E	258	HIS
1	F	61	ASN
1	F	77	ASN
1	F	170	GLN
1	F	196	HIS
1	F	258	HIS
1	G	61	ASN
1	G	77	ASN
1	G	258	HIS
1	H	61	ASN
1	H	77	ASN
1	H	170	GLN
1	H	196	HIS
1	H	255	HIS
1	H	258	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	283/301 (94%)	-0.06	16 (5%)	27	24	69, 118, 193, 227	0
1	B	283/301 (94%)	-0.18	10 (3%)	48	41	66, 116, 187, 258	0
1	C	283/301 (94%)	-0.18	10 (3%)	48	41	68, 111, 189, 233	0
1	D	283/301 (94%)	-0.17	11 (3%)	43	38	64, 108, 199, 270	0
1	E	283/301 (94%)	-0.04	14 (4%)	33	28	67, 113, 194, 252	0
1	F	283/301 (94%)	-0.15	13 (4%)	36	31	65, 114, 200, 250	0
1	G	283/301 (94%)	-0.08	16 (5%)	27	24	66, 114, 207, 297	0
1	H	283/301 (94%)	-0.08	12 (4%)	40	34	73, 116, 197, 239	0
All	All	2264/2408 (94%)	-0.12	102 (4%)	37	32	64, 114, 197, 297	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	280	ASP	5.8
1	G	107	PRO	5.0
1	D	280	ASP	4.7
1	C	12	PRO	4.4
1	E	298	HIS	4.3
1	G	220	HIS	4.1
1	E	282	ARG	4.0
1	H	81	GLY	3.9
1	B	280	ASP	3.9
1	B	281	GLY	3.9
1	B	282	ARG	3.9
1	A	35	ASP	3.8
1	G	281	GLY	3.8
1	D	33	TRP	3.7
1	A	298	HIS	3.7
1	E	220	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	234	ASN	3.7
1	E	280	ASP	3.6
1	H	35	ASP	3.6
1	F	35	ASP	3.6
1	D	299	HIS	3.5
1	A	187	GLN	3.5
1	G	282	ARG	3.4
1	D	71	CYS	3.3
1	F	12	PRO	3.3
1	D	277	THR	3.2
1	C	280	ASP	3.2
1	A	81	GLY	3.1
1	H	16	ASN	3.1
1	E	35	ASP	3.1
1	D	279	PRO	3.0
1	A	280	ASP	2.9
1	G	73	ASP	2.9
1	B	279	PRO	2.9
1	A	12	PRO	2.8
1	C	298	HIS	2.8
1	A	71	CYS	2.8
1	F	280	ASP	2.8
1	F	73	ASP	2.8
1	A	73	ASP	2.7
1	G	277	THR	2.7
1	F	76	GLU	2.7
1	F	236	HIS	2.7
1	C	82	SER	2.7
1	E	299	HIS	2.7
1	E	77	ASN	2.7
1	G	27	GLY	2.7
1	G	279	PRO	2.6
1	E	279	PRO	2.6
1	D	282	ARG	2.6
1	A	188	GLU	2.6
1	E	101	LYS	2.6
1	E	80	PRO	2.6
1	C	81	GLY	2.6
1	F	279	PRO	2.6
1	H	12	PRO	2.6
1	E	73	ASP	2.6
1	F	187	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	18	ASP	2.5
1	B	33	TRP	2.5
1	H	280	ASP	2.5
1	A	16	ASN	2.5
1	D	220	HIS	2.4
1	C	18	ASP	2.4
1	C	187	GLN	2.4
1	E	12	PRO	2.4
1	E	277	THR	2.4
1	G	71	CYS	2.4
1	B	298	HIS	2.4
1	G	284	ALA	2.4
1	B	236	HIS	2.4
1	G	298	HIS	2.4
1	H	234	ASN	2.3
1	B	234	ASN	2.3
1	A	268	GLY	2.3
1	D	278	LEU	2.3
1	A	279	PRO	2.3
1	H	80	PRO	2.2
1	F	18	ASP	2.2
1	F	33	TRP	2.2
1	A	189	GLY	2.2
1	C	80	PRO	2.2
1	H	70	ALA	2.2
1	D	284	ALA	2.2
1	F	16	ASN	2.2
1	H	299	HIS	2.2
1	G	236	HIS	2.1
1	F	81	GLY	2.1
1	H	279	PRO	2.1
1	B	77	ASN	2.1
1	D	35	ASP	2.1
1	A	33	TRP	2.1
1	C	234	ASN	2.1
1	G	35	ASP	2.1
1	F	298	HIS	2.1
1	H	33	TRP	2.1
1	C	13	ARG	2.1
1	H	71	CYS	2.0
1	B	79	ARG	2.0
1	G	76	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	34	LEU	2.0
1	E	33	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	K	C	1300	1/1	0.61	0.27	1.74	159,159,159,159	0
2	K	F	1301	1/1	0.92	0.18	0.24	159,159,159,159	0
2	K	A	1301	1/1	0.85	0.14	-0.58	144,144,144,144	0
2	K	H	1300	1/1	0.91	0.21	-0.78	145,145,145,145	0
2	K	F	1300	1/1	0.72	0.10	-2.20	128,128,128,128	0
2	K	A	1300	1/1	0.87	0.10	-2.49	149,149,149,149	0

6.5 Other polymers (i)

There are no such residues in this entry.