Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 07:24 PM EDT

PDB ID	:	3O9U
Title	:	Effector domain of influenza A/PR/8/34 NS1
Authors	:	Kerry, P.S.; Lewis, A.; Hale, B.G.; Hass, C.; Taylor, M.A.; Randall, R.E.; Russell, R.J.M.
Deposited on	:	2010-08-04
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

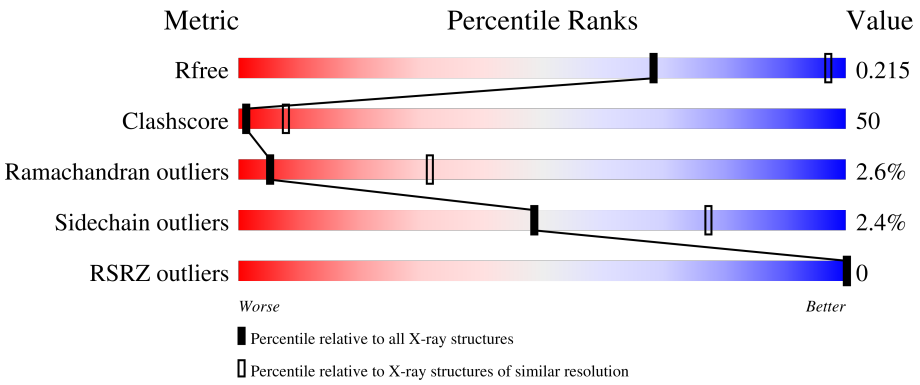
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	152	28% 45% • 24%
1	B	152	28% 45% • 24%
1	C	152	28% 45% • 24%
1	D	152	27% 45% • • 24%
1	E	152	27% 46% • 24%

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Mol	Chain	Length	Quality of chain
1	F	152	28% 43% • 25%
1	G	152	28% 45% • 24%
1	H	152	29% 45% • 24%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7247 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 Nonstructural protein 1.

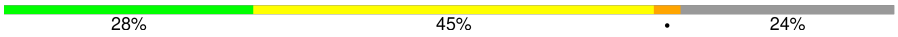
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	116	908	577	154	171	6	1	0	0
			Total	C	N	O	S			
1	A	116	908	577	154	171	6	1	0	0
			Total	C	N	O	S			
1	C	116	908	577	154	171	6	1	0	0
			Total	C	N	O	S			
1	D	116	908	577	154	171	6	0	0	0
			Total	C	N	O	S			
1	E	116	908	577	154	171	6	0	0	0
			Total	C	N	O	S			
1	F	114	891	568	149	168	6	0	0	0
			Total	C	N	O	S			
1	G	116	908	577	154	171	6	1	0	0
			Total	C	N	O	S			
1	H	116	908	577	154	171	6	1	0	0

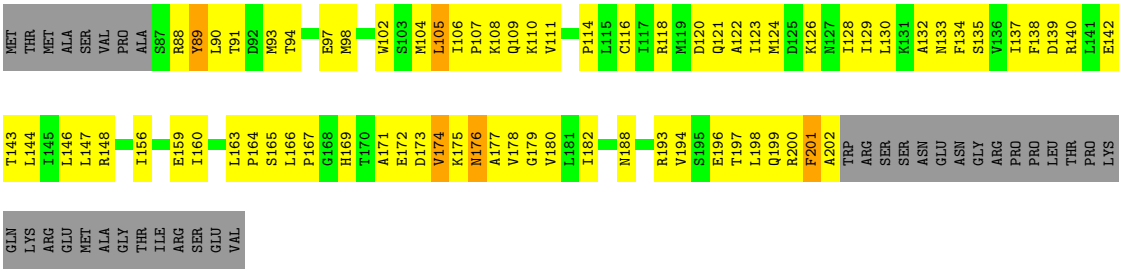
3 Residue-property plots (i)

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

• Molecule 1: Nonstructural protein 1

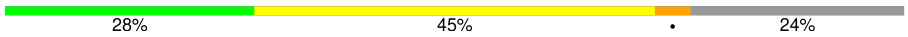
Chain B:

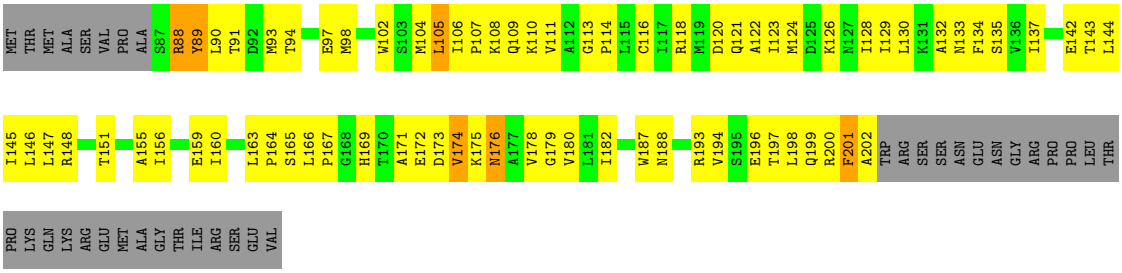




• Molecule 1: Nonstructural protein 1

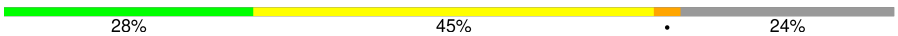
Chain A:

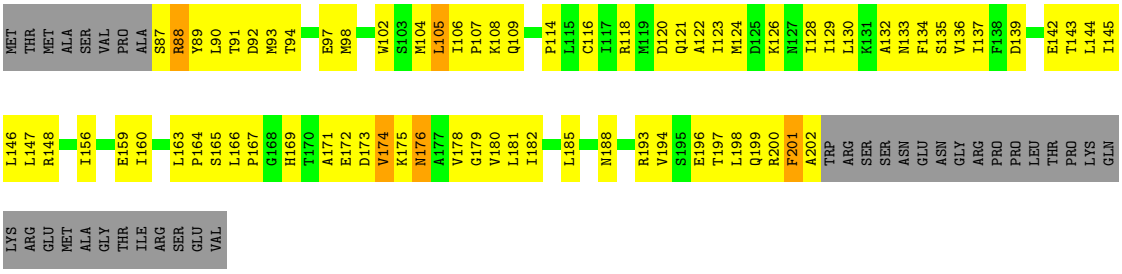




• Molecule 1: Nonstructural protein 1

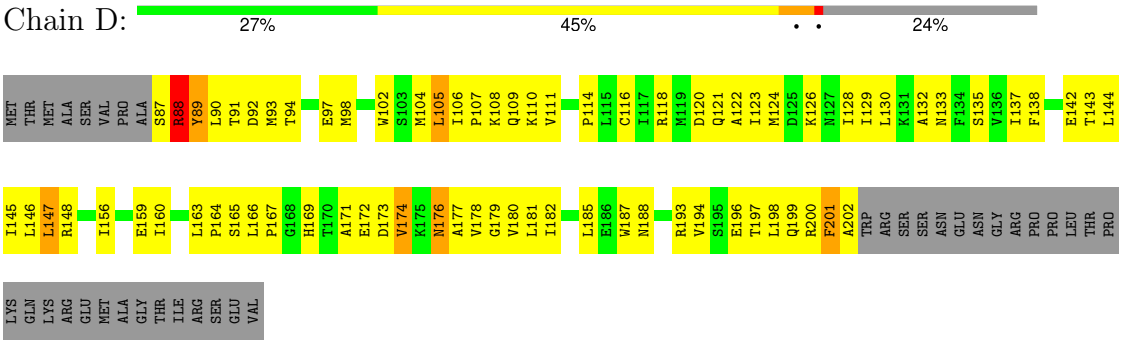
Chain C:





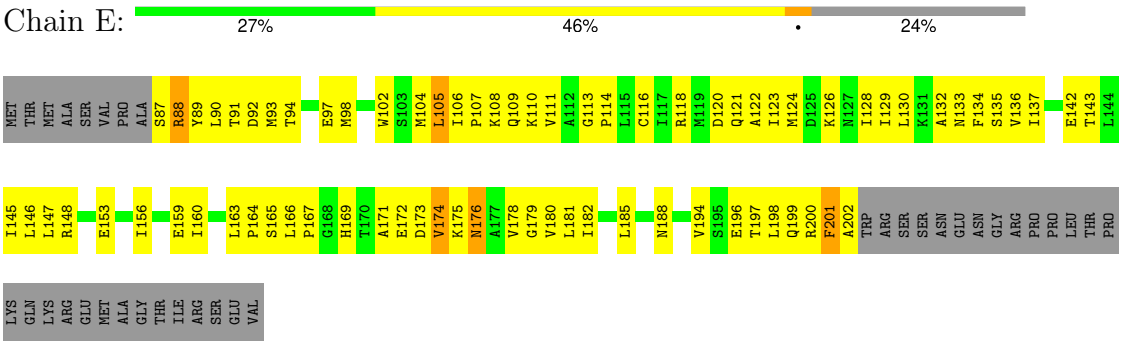
• Molecule 1: Nonstructural protein 1

Chain D:



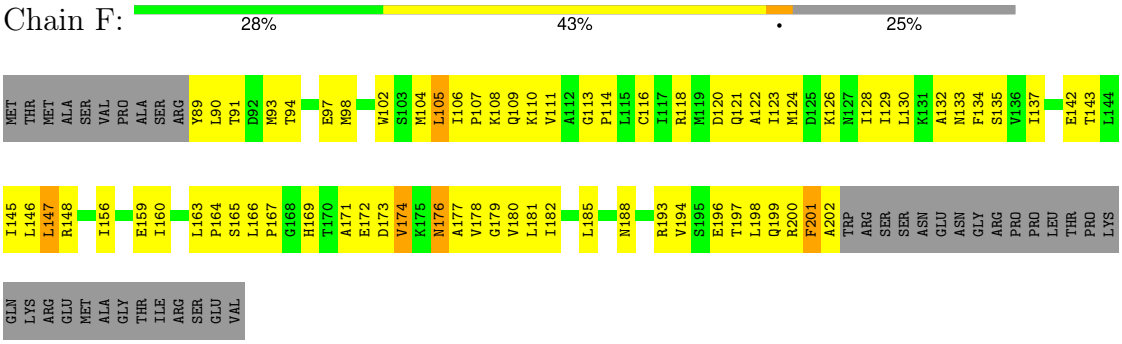
- Molecule 1: Nonstructural protein 1

Chain E:



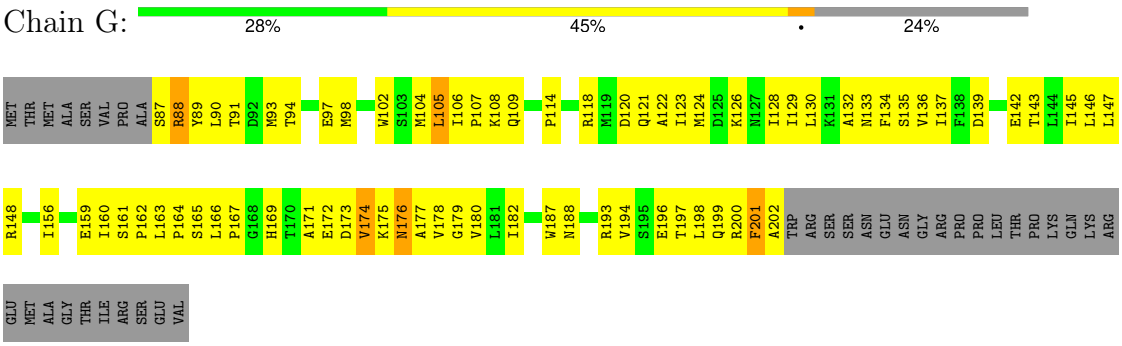
- Molecule 1: Nonstructural protein 1

Chain F:



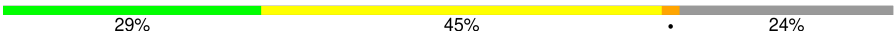
- Molecule 1: Nonstructural protein 1

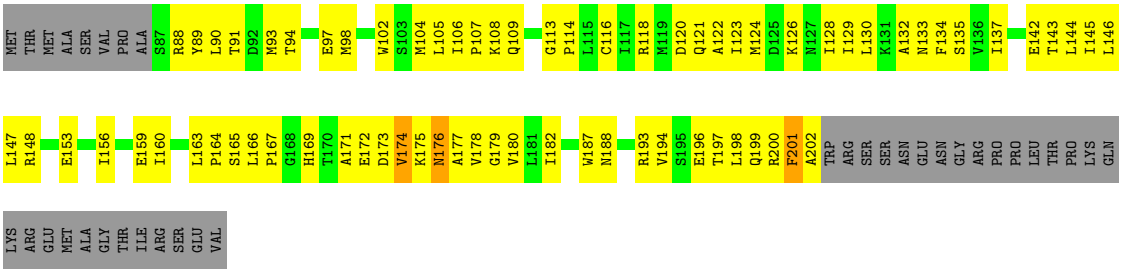
Chain G:



- Molecule 1: Nonstructural protein 1

Chain H:


29%
45%
•
24%


MET THR MET ALA SER VAL PRO ALA S87 R88 Y89 L90 T91 D92 M93 T94 E97 M98 W102 S103 M104 L105 I106 P107 K108 Q109 G113 P114 L115 C116 I117 R118 M119 D120 Q121 A122 I123 M124 D125 K126 N127 I128 I129 L130 K131 A132 N133 F134 S135 V136 I137 E142 T143 L144 I145 L146
L147 R148 E153 I156 E159 I160 L163 P164 S165 L166 P167 G168 H169 T170 A171 E172 D173 V174 K175 N176 A177 V178 G179 V180 L181 I182 W187 N188 R193 V194 S195 E196 T197 L198 Q199 R200 F201 A202 TRP ARG SER SER ASN GLU ASN GLY ARG PRO PRO LEU THR PRO LYS GLN
LYS ARG GLU MET ALA GLY THR ILE ARG SER GLU VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	114.12Å 114.12Å 199.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.87 – 3.20 19.87 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.87-3.20) 97.9 (19.87-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.174 , 0.222 0.175 , 0.215	Depositor DCC
R_{free} test set	1208 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	79.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.439 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7247	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.43	0/922	0.62	0/1248
1	B	0.45	0/922	0.62	0/1248
1	C	0.48	0/922	0.62	0/1248
1	D	0.41	0/922	0.63	0/1248
1	E	0.44	0/922	0.62	0/1248
1	F	0.39	0/905	0.61	0/1226
1	G	0.40	0/922	0.61	0/1248
1	H	0.39	0/922	0.60	0/1248
All	All	0.42	0/7359	0.62	0/9962

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	908	0	929	98	0
1	B	908	0	929	101	0
1	C	908	0	929	100	0
1	D	908	0	929	90	0
1	E	908	0	929	95	0
1	F	891	0	911	92	0
1	G	908	0	929	96	0
1	H	908	0	929	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7247	0	7414	732	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 50.

All (732) 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:90:LEU:HD12	1:A:91:THR:H	1.19	1.06
1:E:200:ARG:HD3	1:H:106:ILE:HD11	1.11	1.06
1:B:140:ARG:HB2	1:A:124:MET:SD	1.97	1.03
1:B:90:LEU:HD12	1:B:91:THR:H	1.19	1.02
1:G:90:LEU:HD12	1:G:91:THR:H	1.24	1.02
1:F:90:LEU:HD12	1:F:91:THR:H	1.22	1.01
1:E:87:SER:O	1:E:88:ARG:HG2	1.57	1.00
1:E:200:ARG:CD	1:H:106:ILE:HD11	1.92	1.00
1:F:130:LEU:HB3	1:F:147:LEU:HD11	1.44	1.00
1:H:90:LEU:HD12	1:H:91:THR:H	1.24	0.99
1:E:90:LEU:HD12	1:E:91:THR:H	1.25	0.98
1:D:90:LEU:HD12	1:D:91:THR:H	1.28	0.98
1:G:88:ARG:HB2	1:G:136:VAL:O	1.65	0.96
1:E:130:LEU:HB3	1:E:147:LEU:HD11	1.45	0.95
1:H:130:LEU:HB3	1:H:147:LEU:HD11	1.48	0.95
1:D:130:LEU:HB3	1:D:147:LEU:HD11	1.48	0.94
1:G:130:LEU:HB3	1:G:147:LEU:HD11	1.49	0.93
1:C:90:LEU:HD12	1:C:91:THR:H	1.30	0.92
1:B:138:PHE:CE1	1:C:109:GLN:HB2	2.04	0.92
1:C:130:LEU:HB3	1:C:147:LEU:HD11	1.52	0.92
1:A:130:LEU:HB3	1:A:147:LEU:HD11	1.51	0.92
1:D:187:TRP:CH2	1:G:108:LYS:HB3	2.05	0.91
1:B:130:LEU:HB3	1:B:147:LEU:HD11	1.54	0.89
1:D:88:ARG:O	1:D:89:TYR:HB3	1.72	0.88
1:E:200:ARG:HD3	1:H:106:ILE:CD1	2.05	0.82
1:C:108:LYS:HD2	1:C:121:GLN:NE2	1.96	0.80
1:B:90:LEU:HD12	1:B:91:THR:N	1.98	0.77
1:C:109:GLN:HG2	1:C:118:ARG:HG2	1.67	0.77
1:B:89:TYR:OH	1:B:133:ASN:HB3	1.83	0.76
1:D:109:GLN:HG2	1:D:118:ARG:HG2	1.67	0.76
1:F:89:TYR:OH	1:F:133:ASN:HB3	1.85	0.76
1:G:109:GLN:HG2	1:G:118:ARG:HG2	1.66	0.76
1:B:139:ASP:O	1:A:122:ALA:HA	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ILE:HG13	1:F:122:ALA:HB2	1.68	0.76
1:A:90:LEU:HD12	1:A:91:THR:N	1.99	0.75
1:C:89:TYR:OH	1:C:133:ASN:HB3	1.87	0.75
1:G:89:TYR:OH	1:G:133:ASN:HB3	1.86	0.75
1:D:89:TYR:OH	1:D:133:ASN:HB3	1.86	0.75
1:E:109:GLN:HG2	1:E:118:ARG:HG2	1.69	0.75
1:F:90:LEU:HD12	1:F:91:THR:N	2.02	0.75
1:A:90:LEU:CD1	1:A:91:THR:H	1.98	0.75
1:B:137:ILE:HD12	1:B:142:GLU:HG2	1.69	0.74
1:E:89:TYR:OH	1:E:133:ASN:HB3	1.88	0.74
1:B:108:LYS:HD2	1:B:121:GLN:NE2	2.03	0.74
1:H:90:LEU:HD12	1:H:91:THR:N	2.02	0.74
1:H:89:TYR:OH	1:H:133:ASN:HB3	1.87	0.73
1:G:178:VAL:HG12	1:G:182:ILE:HD11	1.70	0.73
1:F:109:GLN:HG2	1:F:118:ARG:HG2	1.69	0.73
1:B:109:GLN:HG2	1:B:118:ARG:HG2	1.70	0.71
1:D:88:ARG:O	1:D:89:TYR:CB	2.37	0.71
1:F:178:VAL:HG12	1:F:182:ILE:HD11	1.71	0.71
1:A:89:TYR:OH	1:A:133:ASN:HB3	1.90	0.71
1:G:90:LEU:HD12	1:G:91:THR:N	2.03	0.70
1:H:178:VAL:HG12	1:H:182:ILE:HD11	1.73	0.70
1:C:178:VAL:HG12	1:C:182:ILE:HD11	1.73	0.70
1:E:91:THR:HA	1:E:133:ASN:CG	2.12	0.70
1:C:137:ILE:HD12	1:C:142:GLU:HG2	1.73	0.70
1:C:88:ARG:HB3	1:C:136:VAL:O	1.92	0.70
1:A:124:MET:HG2	1:A:188:ASN:HB3	1.74	0.69
1:H:90:LEU:CD1	1:H:91:THR:H	2.03	0.69
1:D:137:ILE:HD12	1:D:142:GLU:HG2	1.74	0.69
1:A:178:VAL:HG12	1:A:182:ILE:HD11	1.74	0.69
1:F:137:ILE:HD12	1:F:142:GLU:HG2	1.72	0.69
1:H:109:GLN:HG2	1:H:118:ARG:HG2	1.73	0.69
1:E:90:LEU:HD12	1:E:91:THR:N	2.04	0.69
1:A:109:GLN:HG2	1:A:118:ARG:HG2	1.75	0.68
1:B:178:VAL:HG12	1:B:182:ILE:HD11	1.74	0.68
1:C:106:ILE:HG13	1:C:122:ALA:HB2	1.76	0.68
1:D:106:ILE:HG13	1:D:122:ALA:HB2	1.74	0.68
1:G:137:ILE:HD12	1:G:142:GLU:HG2	1.75	0.68
1:B:90:LEU:CD1	1:B:91:THR:H	2.02	0.67
1:A:137:ILE:HD12	1:A:142:GLU:HG2	1.76	0.67
1:C:91:THR:HA	1:C:133:ASN:CG	2.15	0.67
1:H:137:ILE:HD12	1:H:142:GLU:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:LYS:HD2	1:G:121:GLN:OE1	1.94	0.67
1:A:108:LYS:HD2	1:A:121:GLN:OE1	1.95	0.67
1:B:106:ILE:HG13	1:B:122:ALA:HB2	1.77	0.67
1:A:91:THR:HA	1:A:133:ASN:CG	2.14	0.67
1:D:178:VAL:HG12	1:D:182:ILE:HD11	1.76	0.67
1:A:106:ILE:HG13	1:A:122:ALA:HB2	1.77	0.67
1:A:120:ASP:O	1:A:123:ILE:HG12	1.94	0.66
1:E:178:VAL:HG12	1:E:182:ILE:HD11	1.77	0.66
1:E:137:ILE:HD12	1:E:142:GLU:HG2	1.77	0.66
1:G:106:ILE:HG13	1:G:122:ALA:HB2	1.77	0.66
1:G:174:VAL:O	1:G:178:VAL:HG23	1.95	0.66
1:E:106:ILE:HG13	1:E:122:ALA:HB2	1.78	0.66
1:H:106:ILE:HG13	1:H:122:ALA:HB2	1.77	0.66
1:E:91:THR:HB	1:E:133:ASN:ND2	2.11	0.65
1:D:91:THR:HA	1:D:133:ASN:CG	2.16	0.65
1:F:124:MET:HG2	1:F:188:ASN:HB3	1.79	0.65
1:H:91:THR:HA	1:H:133:ASN:CG	2.16	0.65
1:F:91:THR:HA	1:F:133:ASN:CG	2.17	0.65
1:F:104:MET:HG2	1:F:120:ASP:HB2	1.78	0.65
1:E:148:ARG:HG2	1:E:159:GLU:HB2	1.79	0.65
1:B:140:ARG:CB	1:A:124:MET:SD	2.80	0.64
1:D:90:LEU:HD12	1:D:91:THR:N	2.07	0.64
1:E:124:MET:HG2	1:E:188:ASN:HB3	1.79	0.64
1:G:124:MET:HG2	1:G:188:ASN:HB3	1.78	0.64
1:B:89:TYR:OH	1:B:133:ASN:CB	2.46	0.64
1:B:124:MET:HG2	1:B:188:ASN:HB3	1.79	0.64
1:A:91:THR:HB	1:A:133:ASN:ND2	2.13	0.64
1:H:108:LYS:HD2	1:H:121:GLN:OE1	1.98	0.64
1:C:179:GLY:HA2	1:C:182:ILE:HD12	1.78	0.64
1:E:108:LYS:HD2	1:E:121:GLN:OE1	1.97	0.64
1:F:143:THR:HG23	1:F:169:HIS:CE1	2.33	0.64
1:B:91:THR:HA	1:B:133:ASN:CG	2.18	0.64
1:G:91:THR:HA	1:G:133:ASN:CG	2.18	0.64
1:C:146:LEU:HD11	1:C:159:GLU:HG3	1.80	0.64
1:B:179:GLY:HA2	1:B:182:ILE:HD12	1.80	0.63
1:G:90:LEU:CD1	1:G:91:THR:H	2.06	0.63
1:H:179:GLY:HA2	1:H:182:ILE:HD12	1.80	0.63
1:C:90:LEU:HD12	1:C:91:THR:N	2.09	0.63
1:D:90:LEU:CD1	1:D:91:THR:H	2.09	0.63
1:G:179:GLY:HA2	1:G:182:ILE:HD12	1.79	0.63
1:A:143:THR:HG23	1:A:169:HIS:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:LYS:HD2	1:F:121:GLN:OE1	1.99	0.63
1:H:94:THR:O	1:H:98:MET:HG3	1.98	0.63
1:H:91:THR:HB	1:H:133:ASN:ND2	2.14	0.63
1:C:148:ARG:HG2	1:C:159:GLU:HB2	1.80	0.63
1:E:94:THR:O	1:E:98:MET:HG3	1.99	0.63
1:F:89:TYR:OH	1:F:133:ASN:CB	2.47	0.62
1:F:179:GLY:HA2	1:F:182:ILE:HD12	1.82	0.62
1:E:90:LEU:CD1	1:E:91:THR:H	2.08	0.62
1:E:132:ALA:HB3	1:E:198:LEU:HD21	1.81	0.62
1:D:108:LYS:HD2	1:D:121:GLN:OE1	1.98	0.62
1:C:91:THR:HB	1:C:133:ASN:ND2	2.15	0.62
1:E:179:GLY:HA2	1:E:182:ILE:HD12	1.80	0.62
1:F:94:THR:O	1:F:98:MET:HG3	1.99	0.62
1:D:94:THR:O	1:D:98:MET:HG3	1.99	0.62
1:G:120:ASP:O	1:G:123:ILE:HG12	2.00	0.62
1:B:163:LEU:O	1:B:166:LEU:HD23	2.00	0.62
1:E:174:VAL:O	1:E:178:VAL:HG23	2.00	0.62
1:D:91:THR:HB	1:D:133:ASN:ND2	2.14	0.62
1:H:120:ASP:O	1:H:123:ILE:HG12	2.00	0.62
1:B:108:LYS:HE3	1:E:121:GLN:HE22	1.65	0.61
1:A:94:THR:O	1:A:98:MET:HG3	1.99	0.61
1:C:120:ASP:O	1:C:123:ILE:HG12	2.00	0.61
1:C:124:MET:HG2	1:C:188:ASN:HB3	1.81	0.61
1:C:143:THR:HG23	1:C:169:HIS:CE1	2.35	0.61
1:D:124:MET:HG2	1:D:188:ASN:HB3	1.81	0.61
1:G:163:LEU:O	1:G:166:LEU:HD23	2.00	0.61
1:C:90:LEU:CD1	1:C:91:THR:H	2.09	0.61
1:A:91:THR:HB	1:A:133:ASN:HD21	1.66	0.61
1:C:94:THR:O	1:C:98:MET:HG3	2.01	0.61
1:E:87:SER:O	1:E:88:ARG:CG	2.43	0.61
1:H:132:ALA:HB3	1:H:198:LEU:HD21	1.83	0.61
1:D:120:ASP:O	1:D:123:ILE:HG12	2.01	0.61
1:F:90:LEU:CD1	1:F:91:THR:H	2.04	0.61
1:F:91:THR:HB	1:F:133:ASN:ND2	2.16	0.61
1:G:194:VAL:HG13	1:G:198:LEU:HB2	1.83	0.61
1:E:120:ASP:O	1:E:123:ILE:HG12	2.00	0.61
1:G:148:ARG:HD3	1:G:156:ILE:HD13	1.83	0.60
1:D:194:VAL:HG13	1:D:198:LEU:HB2	1.83	0.60
1:C:89:TYR:OH	1:C:133:ASN:CB	2.49	0.60
1:G:104:MET:HG2	1:G:120:ASP:HB2	1.82	0.60
1:B:120:ASP:O	1:B:123:ILE:HG12	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:O	1:A:89:TYR:HB2	2.00	0.60
1:A:194:VAL:HG13	1:A:198:LEU:HB2	1.82	0.60
1:G:143:THR:HG23	1:G:169:HIS:CE1	2.36	0.60
1:H:93:MET:O	1:H:98:MET:HE2	2.01	0.60
1:F:120:ASP:O	1:F:123:ILE:HG12	2.00	0.60
1:G:148:ARG:HG2	1:G:159:GLU:HB2	1.84	0.60
1:D:104:MET:HG2	1:D:120:ASP:HB2	1.84	0.60
1:D:146:LEU:HD11	1:D:159:GLU:HG3	1.84	0.60
1:E:89:TYR:OH	1:E:133:ASN:CB	2.50	0.60
1:B:94:THR:O	1:B:98:MET:HG3	2.02	0.60
1:C:174:VAL:O	1:C:178:VAL:HG23	2.02	0.60
1:F:163:LEU:O	1:F:166:LEU:HD23	2.02	0.60
1:G:132:ALA:HB3	1:G:198:LEU:HD21	1.84	0.60
1:H:89:TYR:OH	1:H:133:ASN:CB	2.49	0.60
1:H:104:MET:HG2	1:H:120:ASP:HB2	1.84	0.60
1:C:87:SER:O	1:C:88:ARG:HB2	2.01	0.59
1:E:91:THR:HB	1:E:133:ASN:HD21	1.66	0.59
1:D:89:TYR:OH	1:D:133:ASN:CB	2.49	0.59
1:D:148:ARG:HG2	1:D:159:GLU:HB2	1.83	0.59
1:E:194:VAL:HG13	1:E:198:LEU:HB2	1.85	0.59
1:D:174:VAL:O	1:D:178:VAL:HG23	2.02	0.59
1:A:179:GLY:HA2	1:A:182:ILE:HD12	1.84	0.59
1:E:91:THR:HA	1:E:133:ASN:OD1	2.02	0.59
1:C:88:ARG:HG2	1:C:136:VAL:HB	1.82	0.59
1:C:108:LYS:HD2	1:C:121:GLN:HE21	1.66	0.59
1:E:143:THR:HG23	1:E:169:HIS:CE1	2.38	0.59
1:B:105:LEU:O	1:B:107:PRO:HD3	2.03	0.59
1:H:194:VAL:HG13	1:H:198:LEU:HB2	1.84	0.59
1:A:148:ARG:HG2	1:A:159:GLU:HB2	1.85	0.59
1:G:89:TYR:OH	1:G:133:ASN:CB	2.49	0.59
1:A:89:TYR:OH	1:A:133:ASN:CB	2.51	0.58
1:B:146:LEU:HD11	1:B:159:GLU:HG3	1.84	0.58
1:A:102:TRP:CE3	1:A:156:ILE:HG22	2.39	0.58
1:D:187:TRP:CH2	1:G:108:LYS:HE2	2.38	0.58
1:H:124:MET:HG2	1:H:188:ASN:HB3	1.84	0.58
1:B:174:VAL:O	1:B:178:VAL:HG23	2.03	0.58
1:G:91:THR:HB	1:G:133:ASN:ND2	2.18	0.58
1:H:143:THR:HG23	1:H:169:HIS:CE1	2.38	0.58
1:E:104:MET:HG2	1:E:120:ASP:HB2	1.84	0.58
1:E:171:ALA:O	1:E:174:VAL:HB	2.04	0.58
1:H:174:VAL:O	1:H:178:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:TRP:CZ2	1:G:108:LYS:HE2	2.39	0.58
1:F:174:VAL:O	1:F:178:VAL:HG23	2.04	0.58
1:A:163:LEU:O	1:A:166:LEU:HD23	2.04	0.57
1:F:93:MET:O	1:F:98:MET:HE2	2.04	0.57
1:H:163:LEU:O	1:H:166:LEU:HD23	2.04	0.57
1:B:148:ARG:HG2	1:B:159:GLU:HB2	1.85	0.57
1:C:194:VAL:HG13	1:C:198:LEU:HB2	1.85	0.57
1:B:143:THR:HG23	1:B:169:HIS:CE1	2.39	0.57
1:D:148:ARG:HD3	1:D:156:ILE:HD13	1.87	0.57
1:F:194:VAL:HG13	1:F:198:LEU:HB2	1.85	0.57
1:G:94:THR:O	1:G:98:MET:HG3	2.05	0.57
1:B:91:THR:HB	1:B:133:ASN:ND2	2.20	0.57
1:C:104:MET:HG2	1:C:120:ASP:HB2	1.87	0.57
1:B:91:THR:HA	1:B:133:ASN:OD1	2.04	0.57
1:D:187:TRP:CZ2	1:G:108:LYS:HB3	2.39	0.57
1:A:91:THR:HA	1:A:133:ASN:OD1	2.04	0.57
1:H:91:THR:HB	1:H:133:ASN:HD21	1.70	0.57
1:B:106:ILE:HG21	1:B:121:GLN:HB3	1.85	0.57
1:B:164:PRO:O	1:B:166:LEU:HG	2.05	0.57
1:A:114:PRO:HB3	1:A:167:PRO:HB2	1.85	0.57
1:D:143:THR:HG23	1:D:169:HIS:CE1	2.40	0.57
1:D:163:LEU:O	1:D:166:LEU:HD23	2.05	0.57
1:E:163:LEU:O	1:E:166:LEU:HD23	2.05	0.57
1:A:128:ILE:HG22	1:A:129:ILE:N	2.21	0.56
1:A:174:VAL:O	1:A:178:VAL:HG23	2.05	0.56
1:G:105:LEU:HG	1:G:120:ASP:OD2	2.05	0.56
1:E:146:LEU:HD11	1:E:159:GLU:HG3	1.86	0.56
1:H:91:THR:HA	1:H:133:ASN:OD1	2.05	0.56
1:H:146:LEU:HD11	1:H:159:GLU:HG3	1.86	0.56
1:H:148:ARG:HD3	1:H:156:ILE:HD13	1.87	0.56
1:F:148:ARG:HG2	1:F:159:GLU:HB2	1.87	0.56
1:D:114:PRO:HB3	1:D:167:PRO:HB2	1.87	0.56
1:G:164:PRO:O	1:G:166:LEU:HG	2.06	0.56
1:G:146:LEU:HD11	1:G:159:GLU:HG3	1.87	0.56
1:B:194:VAL:HG13	1:B:198:LEU:HB2	1.86	0.56
1:D:91:THR:HA	1:D:133:ASN:OD1	2.06	0.56
1:D:91:THR:HB	1:D:133:ASN:HD21	1.69	0.56
1:B:159:GLU:HG2	1:B:160:ILE:N	2.19	0.56
1:C:91:THR:HB	1:C:133:ASN:HD21	1.70	0.56
1:F:146:LEU:HD11	1:F:159:GLU:HG3	1.87	0.56
1:B:105:LEU:HG	1:B:120:ASP:OD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HG13	1:A:130:LEU:N	2.21	0.55
1:C:159:GLU:HG2	1:C:160:ILE:N	2.21	0.55
1:D:124:MET:O	1:D:126:LYS:HG2	2.06	0.55
1:H:159:GLU:HG2	1:H:160:ILE:N	2.21	0.55
1:F:105:LEU:O	1:F:107:PRO:HD3	2.06	0.55
1:E:114:PRO:HB3	1:E:167:PRO:HB2	1.89	0.55
1:E:159:GLU:HG2	1:E:160:ILE:N	2.21	0.55
1:F:114:PRO:HB3	1:F:167:PRO:HB2	1.88	0.55
1:F:159:GLU:HG2	1:F:160:ILE:N	2.21	0.55
1:B:89:TYR:CZ	1:B:133:ASN:HB3	2.41	0.55
1:C:163:LEU:O	1:C:166:LEU:HD23	2.07	0.55
1:H:148:ARG:HG2	1:H:159:GLU:HB2	1.86	0.55
1:A:104:MET:HG2	1:A:120:ASP:HB2	1.89	0.55
1:A:121:GLN:NE2	1:C:108:LYS:HE3	2.22	0.55
1:B:114:PRO:HB3	1:B:167:PRO:HB2	1.89	0.55
1:A:105:LEU:HG	1:A:120:ASP:OD2	2.07	0.55
1:A:146:LEU:HD11	1:A:159:GLU:HG3	1.88	0.55
1:C:148:ARG:HD3	1:C:156:ILE:HD13	1.89	0.55
1:B:138:PHE:CD1	1:C:109:GLN:HB2	2.42	0.54
1:E:128:ILE:HG22	1:E:129:ILE:N	2.21	0.54
1:B:106:ILE:CG2	1:B:121:GLN:HB3	2.37	0.54
1:C:105:LEU:HG	1:C:120:ASP:OD2	2.07	0.54
1:C:91:THR:HA	1:C:133:ASN:OD1	2.08	0.54
1:F:106:ILE:HG21	1:F:121:GLN:HB3	1.89	0.54
1:D:179:GLY:HA2	1:D:182:ILE:HD12	1.90	0.54
1:B:104:MET:HG2	1:B:120:ASP:HB2	1.90	0.54
1:H:105:LEU:O	1:H:107:PRO:HD3	2.08	0.54
1:C:197:THR:O	1:C:200:ARG:HB3	2.08	0.54
1:E:148:ARG:HD3	1:E:156:ILE:HD13	1.89	0.54
1:E:88:ARG:HB2	1:E:136:VAL:O	2.07	0.54
1:C:114:PRO:HB3	1:C:167:PRO:HB2	1.89	0.54
1:G:91:THR:HA	1:G:133:ASN:OD1	2.08	0.54
1:D:132:ALA:HB3	1:D:198:LEU:HD21	1.90	0.54
1:E:124:MET:O	1:E:126:LYS:HG2	2.08	0.54
1:H:114:PRO:HB3	1:H:167:PRO:HB2	1.89	0.54
1:B:148:ARG:HD3	1:B:156:ILE:HD13	1.90	0.53
1:C:129:ILE:HG13	1:C:130:LEU:N	2.23	0.53
1:H:89:TYR:CZ	1:H:133:ASN:HB3	2.44	0.53
1:H:105:LEU:HG	1:H:120:ASP:OD2	2.07	0.53
1:B:132:ALA:HB3	1:B:198:LEU:HD21	1.90	0.53
1:C:105:LEU:O	1:C:107:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HG	1:D:120:ASP:OD2	2.08	0.53
1:D:164:PRO:O	1:D:166:LEU:HG	2.08	0.53
1:F:91:THR:HA	1:F:133:ASN:OD1	2.09	0.53
1:G:89:TYR:CZ	1:G:133:ASN:HB3	2.43	0.53
1:G:106:ILE:HG21	1:G:121:GLN:HB3	1.91	0.53
1:A:132:ALA:HB3	1:A:198:LEU:HD21	1.91	0.53
1:F:132:ALA:HB3	1:F:198:LEU:HD21	1.91	0.53
1:G:124:MET:O	1:G:126:LYS:HG2	2.09	0.53
1:H:129:ILE:HG13	1:H:130:LEU:N	2.23	0.53
1:E:105:LEU:HG	1:E:120:ASP:OD2	2.08	0.53
1:F:89:TYR:CZ	1:F:133:ASN:HB3	2.44	0.53
1:G:91:THR:HB	1:G:133:ASN:HD21	1.74	0.53
1:D:89:TYR:CZ	1:D:133:ASN:HB3	2.44	0.53
1:B:138:PHE:CZ	1:C:109:GLN:HG3	2.44	0.52
1:B:147:LEU:HG	1:B:148:ARG:N	2.24	0.52
1:C:171:ALA:O	1:C:174:VAL:HB	2.09	0.52
1:G:159:GLU:HG2	1:G:160:ILE:N	2.23	0.52
1:A:159:GLU:HG2	1:A:160:ILE:N	2.23	0.52
1:C:132:ALA:HB3	1:C:198:LEU:HD21	1.90	0.52
1:C:172:GLU:O	1:C:174:VAL:N	2.43	0.52
1:D:106:ILE:HD12	1:D:122:ALA:HA	1.91	0.52
1:D:196:GLU:O	1:D:199:GLN:HG2	2.09	0.52
1:F:196:GLU:O	1:F:199:GLN:HG2	2.09	0.52
1:A:88:ARG:O	1:A:89:TYR:CB	2.58	0.52
1:D:105:LEU:O	1:D:107:PRO:HD3	2.10	0.52
1:F:106:ILE:CG2	1:F:121:GLN:HB3	2.39	0.52
1:F:110:LYS:HE2	1:H:187:TRP:O	2.09	0.52
1:F:164:PRO:O	1:F:166:LEU:HG	2.09	0.52
1:C:89:TYR:CZ	1:C:133:ASN:HB3	2.45	0.52
1:E:89:TYR:CZ	1:E:133:ASN:HB3	2.44	0.52
1:E:102:TRP:CE3	1:E:156:ILE:HG22	2.44	0.52
1:G:106:ILE:HD12	1:G:122:ALA:HA	1.91	0.52
1:C:106:ILE:HD12	1:C:122:ALA:HA	1.90	0.52
1:C:88:ARG:NE	1:C:136:VAL:HG11	2.25	0.52
1:G:114:PRO:HB3	1:G:167:PRO:HB2	1.92	0.52
1:B:91:THR:HB	1:B:133:ASN:HD21	1.74	0.52
1:A:89:TYR:CZ	1:A:133:ASN:HB3	2.45	0.52
1:D:194:VAL:CG1	1:D:198:LEU:HB2	2.40	0.52
1:G:147:LEU:HG	1:G:148:ARG:N	2.24	0.52
1:B:108:LYS:HD2	1:B:121:GLN:HE21	1.74	0.52
1:F:106:ILE:HD12	1:F:122:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ILE:HG21	1:C:121:GLN:HB3	1.91	0.52
1:C:164:PRO:O	1:C:166:LEU:HG	2.10	0.52
1:G:87:SER:OG	1:G:88:ARG:N	2.36	0.51
1:H:176:ASN:O	1:H:180:VAL:HG23	2.10	0.51
1:B:106:ILE:HD12	1:B:122:ALA:HA	1.91	0.51
1:F:128:ILE:HG22	1:F:129:ILE:N	2.25	0.51
1:G:89:TYR:HD1	1:G:135:SER:HA	1.75	0.51
1:H:124:MET:O	1:H:126:LYS:HG2	2.10	0.51
1:C:132:ALA:HB2	1:C:147:LEU:HD12	1.92	0.51
1:E:129:ILE:HG13	1:E:130:LEU:N	2.25	0.51
1:F:91:THR:HB	1:F:133:ASN:HD21	1.73	0.51
1:H:128:ILE:HG22	1:H:129:ILE:N	2.24	0.51
1:B:124:MET:O	1:B:126:LYS:HG2	2.11	0.51
1:G:105:LEU:O	1:G:107:PRO:HD3	2.10	0.51
1:E:105:LEU:O	1:E:107:PRO:HD3	2.11	0.51
1:E:164:PRO:O	1:E:166:LEU:HG	2.10	0.51
1:F:197:THR:O	1:F:200:ARG:HB3	2.10	0.51
1:B:196:GLU:O	1:B:199:GLN:HG2	2.09	0.51
1:A:197:THR:O	1:A:200:ARG:HB3	2.11	0.51
1:D:129:ILE:HG13	1:D:130:LEU:N	2.25	0.51
1:H:196:GLU:O	1:H:199:GLN:HG2	2.11	0.51
1:F:147:LEU:HG	1:F:148:ARG:N	2.26	0.51
1:H:194:VAL:CG1	1:H:198:LEU:HB2	2.40	0.51
1:B:172:GLU:O	1:B:174:VAL:N	2.44	0.51
1:C:179:GLY:CA	1:C:182:ILE:HD12	2.41	0.51
1:G:129:ILE:HG13	1:G:130:LEU:N	2.25	0.51
1:B:128:ILE:HG22	1:B:129:ILE:N	2.26	0.51
1:E:172:GLU:O	1:E:173:ASP:C	2.49	0.51
1:B:129:ILE:HG13	1:B:130:LEU:N	2.26	0.50
1:A:147:LEU:HG	1:A:148:ARG:N	2.25	0.50
1:H:171:ALA:O	1:H:174:VAL:HB	2.11	0.50
1:B:108:LYS:HE3	1:E:121:GLN:NE2	2.25	0.50
1:D:159:GLU:HG2	1:D:160:ILE:N	2.26	0.50
1:F:172:GLU:O	1:F:173:ASP:C	2.50	0.50
1:G:88:ARG:HH12	1:G:139:ASP:CG	2.13	0.50
1:G:106:ILE:CG2	1:G:121:GLN:HB3	2.41	0.50
1:F:148:ARG:HD3	1:F:156:ILE:HD13	1.92	0.50
1:A:105:LEU:O	1:A:107:PRO:HD3	2.11	0.50
1:F:124:MET:O	1:F:126:LYS:HG2	2.10	0.50
1:E:196:GLU:O	1:E:199:GLN:HG2	2.11	0.50
1:G:128:ILE:HG22	1:G:129:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:SER:OG	1:B:167:PRO:HD3	2.12	0.50
1:E:106:ILE:HD12	1:E:122:ALA:HA	1.93	0.50
1:E:197:THR:O	1:E:200:ARG:HB3	2.11	0.50
1:H:164:PRO:O	1:H:166:LEU:HG	2.12	0.50
1:B:123:ILE:HD13	1:B:123:ILE:N	2.27	0.50
1:A:91:THR:CB	1:A:133:ASN:ND2	2.74	0.50
1:E:106:ILE:HG21	1:E:121:GLN:HB3	1.94	0.50
1:B:139:ASP:OD1	1:A:121:GLN:CD	2.49	0.50
1:A:196:GLU:O	1:A:199:GLN:HG2	2.11	0.50
1:C:128:ILE:HG22	1:C:129:ILE:N	2.26	0.50
1:B:172:GLU:O	1:B:173:ASP:C	2.48	0.50
1:E:91:THR:CB	1:E:133:ASN:ND2	2.74	0.50
1:H:197:THR:O	1:H:200:ARG:HB3	2.12	0.50
1:C:108:LYS:O	1:C:118:ARG:HA	2.12	0.49
1:D:128:ILE:HG22	1:D:129:ILE:N	2.26	0.49
1:D:93:MET:O	1:D:98:MET:HE2	2.12	0.49
1:A:164:PRO:O	1:A:166:LEU:HG	2.13	0.49
1:D:199:GLN:O	1:D:200:ARG:C	2.51	0.49
1:A:106:ILE:HD12	1:A:122:ALA:HA	1.94	0.49
1:D:171:ALA:O	1:D:174:VAL:HB	2.11	0.49
1:D:197:THR:O	1:D:200:ARG:HB3	2.12	0.49
1:F:108:LYS:O	1:F:118:ARG:HA	2.12	0.49
1:G:172:GLU:O	1:G:173:ASP:C	2.50	0.49
1:H:147:LEU:HG	1:H:148:ARG:N	2.28	0.49
1:G:93:MET:O	1:G:98:MET:HE2	2.13	0.49
1:B:93:MET:O	1:B:98:MET:HE2	2.11	0.49
1:D:102:TRP:CE3	1:D:156:ILE:HG22	2.47	0.49
1:C:88:ARG:CZ	1:C:136:VAL:HG11	2.43	0.49
1:C:172:GLU:O	1:C:173:ASP:C	2.50	0.49
1:D:172:GLU:O	1:D:173:ASP:C	2.50	0.49
1:E:147:LEU:HG	1:E:148:ARG:N	2.27	0.49
1:B:138:PHE:CE1	1:C:109:GLN:CB	2.89	0.49
1:B:200:ARG:HH21	1:A:123:ILE:HD12	1.78	0.49
1:C:102:TRP:CE3	1:C:156:ILE:HG22	2.48	0.49
1:A:105:LEU:HD12	1:A:122:ALA:HB3	1.94	0.49
1:G:179:GLY:CA	1:G:182:ILE:HD12	2.42	0.49
1:A:106:ILE:HG21	1:A:121:GLN:HB3	1.94	0.48
1:G:194:VAL:CG1	1:G:198:LEU:HB2	2.42	0.48
1:A:148:ARG:HD3	1:A:156:ILE:HD13	1.95	0.48
1:G:114:PRO:HA	1:G:163:LEU:HD12	1.95	0.48
1:H:179:GLY:CA	1:H:182:ILE:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:CG1	1:A:198:LEU:HB2	2.43	0.48
1:G:171:ALA:O	1:G:174:VAL:HB	2.13	0.48
1:H:106:ILE:HD12	1:H:122:ALA:HA	1.94	0.48
1:C:106:ILE:CG2	1:C:121:GLN:HB3	2.42	0.48
1:C:196:GLU:O	1:C:199:GLN:HG2	2.13	0.48
1:D:106:ILE:HG21	1:D:121:GLN:HB3	1.94	0.48
1:D:129:ILE:HD12	1:D:193:ARG:C	2.34	0.48
1:H:89:TYR:HD1	1:H:135:SER:HA	1.78	0.48
1:H:106:ILE:HG21	1:H:121:GLN:HB3	1.94	0.48
1:A:132:ALA:HB2	1:A:147:LEU:HD12	1.96	0.48
1:A:172:GLU:O	1:A:173:ASP:C	2.51	0.48
1:F:105:LEU:HG	1:F:120:ASP:OD2	2.13	0.48
1:F:194:VAL:CG1	1:F:198:LEU:HB2	2.43	0.48
1:B:197:THR:O	1:B:200:ARG:HB3	2.12	0.48
1:A:123:ILE:N	1:A:123:ILE:HD13	2.29	0.48
1:A:128:ILE:CG2	1:A:129:ILE:N	2.77	0.48
1:G:172:GLU:O	1:G:174:VAL:N	2.47	0.48
1:H:114:PRO:HA	1:H:163:LEU:HD12	1.95	0.48
1:A:129:ILE:HD12	1:A:193:ARG:C	2.34	0.48
1:E:106:ILE:CG2	1:E:121:GLN:HB3	2.44	0.48
1:G:201:PHE:HA	1:G:202:ALA:HA	1.65	0.48
1:F:129:ILE:HG13	1:F:130:LEU:N	2.27	0.48
1:D:114:PRO:HA	1:D:163:LEU:HD12	1.96	0.48
1:E:176:ASN:O	1:E:180:VAL:HG23	2.13	0.48
1:G:172:GLU:C	1:G:174:VAL:N	2.67	0.48
1:H:116:CYS:SG	1:H:118:ARG:CZ	3.02	0.48
1:B:140:ARG:HD2	1:A:124:MET:SD	2.54	0.47
1:C:105:LEU:HG	1:C:105:LEU:H	1.52	0.47
1:D:91:THR:CB	1:D:133:ASN:ND2	2.77	0.47
1:G:108:LYS:O	1:G:118:ARG:HA	2.14	0.47
1:B:105:LEU:HD12	1:B:122:ALA:HB3	1.95	0.47
1:C:91:THR:CB	1:C:133:ASN:ND2	2.77	0.47
1:F:114:PRO:HA	1:F:163:LEU:HD12	1.95	0.47
1:B:171:ALA:O	1:B:174:VAL:HB	2.14	0.47
1:D:108:LYS:CD	1:D:121:GLN:HB2	2.44	0.47
1:D:108:LYS:O	1:D:118:ARG:HA	2.15	0.47
1:B:89:TYR:HD1	1:B:135:SER:HA	1.79	0.47
1:B:114:PRO:HA	1:B:163:LEU:HD12	1.95	0.47
1:B:176:ASN:O	1:B:180:VAL:HG23	2.15	0.47
1:A:199:GLN:O	1:A:200:ARG:C	2.53	0.47
1:C:124:MET:O	1:C:126:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:SER:OG	1:E:167:PRO:HD3	2.15	0.47
1:F:89:TYR:HD1	1:F:135:SER:HA	1.80	0.47
1:F:102:TRP:CE3	1:F:156:ILE:HG22	2.49	0.47
1:G:196:GLU:O	1:G:199:GLN:HG2	2.13	0.47
1:H:172:GLU:O	1:H:173:ASP:C	2.52	0.47
1:G:197:THR:O	1:G:200:ARG:HB3	2.15	0.47
1:B:129:ILE:HD12	1:B:193:ARG:C	2.35	0.47
1:A:89:TYR:HD1	1:A:135:SER:HA	1.80	0.47
1:A:135:SER:HB3	1:A:145:ILE:HD11	1.96	0.47
1:C:88:ARG:NH1	1:C:139:ASP:OD1	2.46	0.47
1:C:194:VAL:CG1	1:C:198:LEU:HB2	2.44	0.47
1:E:194:VAL:CG1	1:E:198:LEU:HB2	2.43	0.47
1:H:123:ILE:N	1:H:123:ILE:HD13	2.29	0.47
1:H:165:SER:OG	1:H:167:PRO:HD3	2.15	0.47
1:B:179:GLY:CA	1:B:182:ILE:HD12	2.44	0.47
1:F:165:SER:OG	1:F:167:PRO:HD3	2.14	0.47
1:H:91:THR:CB	1:H:133:ASN:ND2	2.78	0.47
1:B:194:VAL:CG1	1:B:198:LEU:HB2	2.45	0.47
1:A:134:PHE:HZ	1:A:198:LEU:HD23	1.79	0.47
1:D:147:LEU:HG	1:D:148:ARG:N	2.29	0.47
1:B:116:CYS:HB3	1:B:118:ARG:HH12	1.80	0.47
1:A:121:GLN:HE22	1:C:108:LYS:HE3	1.79	0.47
1:C:114:PRO:HA	1:C:163:LEU:HD12	1.97	0.47
1:G:108:LYS:CD	1:G:121:GLN:HB2	2.44	0.47
1:G:201:PHE:HA	1:G:201:PHE:HD1	1.63	0.47
1:B:134:PHE:HZ	1:B:198:LEU:HD23	1.80	0.46
1:C:89:TYR:HD1	1:C:135:SER:HA	1.79	0.46
1:C:172:GLU:C	1:C:174:VAL:N	2.65	0.46
1:F:134:PHE:HZ	1:F:198:LEU:HD23	1.79	0.46
1:B:93:MET:HA	1:B:97:GLU:OE1	2.15	0.46
1:A:90:LEU:CD1	1:A:91:THR:N	2.71	0.46
1:E:147:LEU:C	1:E:147:LEU:HD23	2.36	0.46
1:E:172:GLU:O	1:E:174:VAL:N	2.48	0.46
1:F:199:GLN:O	1:F:200:ARG:C	2.54	0.46
1:H:172:GLU:O	1:H:174:VAL:N	2.48	0.46
1:B:102:TRP:CE3	1:B:156:ILE:HG22	2.50	0.46
1:C:199:GLN:O	1:C:200:ARG:C	2.53	0.46
1:D:132:ALA:HB2	1:D:147:LEU:HD12	1.98	0.46
1:E:172:GLU:C	1:E:174:VAL:N	2.68	0.46
1:E:201:PHE:HA	1:E:202:ALA:HA	1.65	0.46
1:H:108:LYS:O	1:H:118:ARG:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:LYS:HD2	1:D:121:GLN:HB2	1.98	0.46
1:E:128:ILE:CG2	1:E:129:ILE:N	2.78	0.46
1:G:176:ASN:O	1:G:180:VAL:HG23	2.15	0.46
1:H:106:ILE:CG2	1:H:121:GLN:HB3	2.45	0.46
1:B:201:PHE:HA	1:B:202:ALA:HA	1.65	0.46
1:A:171:ALA:O	1:A:174:VAL:HB	2.15	0.46
1:C:87:SER:O	1:C:88:ARG:CB	2.62	0.46
1:C:116:CYS:HB3	1:C:118:ARG:HH12	1.81	0.46
1:D:106:ILE:CG2	1:D:121:GLN:HB3	2.46	0.46
1:F:108:LYS:CD	1:F:121:GLN:HB2	2.46	0.46
1:F:196:GLU:O	1:F:197:THR:C	2.54	0.46
1:F:110:LYS:CE	1:H:187:TRP:O	2.64	0.46
1:G:108:LYS:HD2	1:G:121:GLN:HB2	1.98	0.46
1:G:129:ILE:HD12	1:G:193:ARG:C	2.35	0.46
1:A:105:LEU:HG	1:A:105:LEU:H	1.53	0.46
1:D:132:ALA:O	1:D:133:ASN:OD1	2.34	0.46
1:F:171:ALA:O	1:F:174:VAL:HB	2.16	0.46
1:G:165:SER:OG	1:G:167:PRO:HD3	2.16	0.46
1:B:132:ALA:HB2	1:B:147:LEU:HD12	1.98	0.46
1:A:176:ASN:O	1:A:180:VAL:HG23	2.15	0.46
1:A:201:PHE:HA	1:A:202:ALA:HA	1.63	0.46
1:C:105:LEU:HD12	1:C:122:ALA:HB3	1.98	0.46
1:E:89:TYR:HD1	1:E:135:SER:HA	1.80	0.46
1:E:114:PRO:HA	1:E:163:LEU:HD12	1.98	0.46
1:H:102:TRP:CE3	1:H:156:ILE:HG22	2.51	0.46
1:C:108:LYS:CD	1:C:121:GLN:HB2	2.46	0.46
1:D:201:PHE:HA	1:D:202:ALA:HA	1.69	0.46
1:F:132:ALA:HB2	1:F:147:LEU:HD12	1.97	0.46
1:F:172:GLU:O	1:F:174:VAL:N	2.49	0.46
1:A:93:MET:O	1:A:98:MET:HE2	2.16	0.45
1:A:172:GLU:O	1:A:174:VAL:N	2.49	0.45
1:D:110:LYS:NZ	1:G:187:TRP:O	2.47	0.45
1:D:172:GLU:O	1:D:174:VAL:N	2.49	0.45
1:E:132:ALA:O	1:E:133:ASN:OD1	2.33	0.45
1:F:201:PHE:HA	1:F:202:ALA:HA	1.67	0.45
1:H:172:GLU:C	1:H:174:VAL:N	2.68	0.45
1:H:199:GLN:O	1:H:200:ARG:C	2.54	0.45
1:D:89:TYR:HD1	1:D:135:SER:HA	1.81	0.45
1:D:92:ASP:N	1:D:133:ASN:OD1	2.44	0.45
1:G:98:MET:CE	1:G:133:ASN:ND2	2.79	0.45
1:H:105:LEU:HD12	1:H:122:ALA:HB3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LYS:O	1:B:118:ARG:HA	2.16	0.45
1:A:113:GLY:HA3	1:A:114:PRO:HD3	1.81	0.45
1:A:114:PRO:HA	1:A:163:LEU:HD12	1.97	0.45
1:A:147:LEU:HD23	1:A:147:LEU:C	2.36	0.45
1:B:172:GLU:C	1:B:174:VAL:N	2.67	0.45
1:A:187:TRP:CZ2	1:C:108:LYS:HB3	2.51	0.45
1:B:199:GLN:O	1:B:200:ARG:C	2.55	0.45
1:C:135:SER:HB3	1:C:145:ILE:HD11	1.97	0.45
1:H:128:ILE:CG2	1:H:129:ILE:N	2.80	0.45
1:B:139:ASP:CG	1:A:121:GLN:CD	2.76	0.45
1:A:106:ILE:CG2	1:A:121:GLN:HB3	2.47	0.45
1:C:133:ASN:O	1:C:144:LEU:HD12	2.17	0.45
1:E:108:LYS:O	1:E:118:ARG:HA	2.17	0.45
1:F:104:MET:HB2	1:F:104:MET:HE3	1.87	0.45
1:F:110:LYS:HG2	1:F:111:VAL:N	2.32	0.45
1:G:132:ALA:HB2	1:G:147:LEU:HD12	1.99	0.45
1:F:106:ILE:CG1	1:F:122:ALA:HB2	2.44	0.45
1:G:105:LEU:HD12	1:G:122:ALA:HB3	1.99	0.45
1:H:116:CYS:SG	1:H:118:ARG:NH1	2.90	0.45
1:B:196:GLU:O	1:B:197:THR:C	2.55	0.45
1:A:174:VAL:O	1:A:175:LYS:C	2.55	0.45
1:F:201:PHE:HA	1:F:201:PHE:HD1	1.66	0.45
1:H:166:LEU:N	1:H:167:PRO:HD3	2.32	0.45
1:A:93:MET:HA	1:A:97:GLU:OE1	2.17	0.44
1:A:108:LYS:O	1:A:118:ARG:HA	2.17	0.44
1:A:124:MET:O	1:A:126:LYS:HG2	2.16	0.44
1:D:123:ILE:N	1:D:123:ILE:HD13	2.32	0.44
1:E:116:CYS:HB3	1:E:118:ARG:HH12	1.81	0.44
1:E:166:LEU:N	1:E:167:PRO:HD3	2.32	0.44
1:F:123:ILE:N	1:F:123:ILE:HD13	2.32	0.44
1:H:98:MET:CE	1:H:133:ASN:ND2	2.80	0.44
1:F:91:THR:CB	1:F:133:ASN:ND2	2.80	0.44
1:F:93:MET:HA	1:F:97:GLU:OE1	2.17	0.44
1:F:179:GLY:CA	1:F:182:ILE:HD12	2.46	0.44
1:G:123:ILE:HD13	1:G:123:ILE:N	2.32	0.44
1:B:147:LEU:C	1:B:147:LEU:HD23	2.38	0.44
1:C:176:ASN:O	1:C:180:VAL:HG23	2.17	0.44
1:E:199:GLN:O	1:E:200:ARG:C	2.56	0.44
1:F:116:CYS:HB3	1:F:118:ARG:HH12	1.82	0.44
1:F:135:SER:HB3	1:F:145:ILE:HD11	1.99	0.44
1:H:132:ALA:HB2	1:H:147:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:O	1:B:89:TYR:HB2	2.17	0.44
1:D:105:LEU:HD12	1:D:122:ALA:HB3	1.99	0.44
1:H:135:SER:HB3	1:H:145:ILE:HD11	1.99	0.44
1:A:198:LEU:O	1:A:201:PHE:N	2.51	0.44
1:C:147:LEU:HG	1:C:148:ARG:N	2.33	0.44
1:D:176:ASN:O	1:D:180:VAL:HG23	2.18	0.44
1:E:113:GLY:HA3	1:E:114:PRO:HD3	1.83	0.44
1:H:93:MET:C	1:H:98:MET:HE2	2.38	0.44
1:A:133:ASN:O	1:A:144:LEU:HD12	2.18	0.44
1:A:165:SER:OG	1:A:167:PRO:HD3	2.17	0.44
1:D:165:SER:OG	1:D:167:PRO:HD3	2.18	0.44
1:D:172:GLU:C	1:D:174:VAL:N	2.70	0.44
1:F:176:ASN:O	1:F:180:VAL:HG23	2.18	0.44
1:C:201:PHE:HA	1:C:202:ALA:HA	1.63	0.44
1:F:108:LYS:HD2	1:F:121:GLN:HB2	1.99	0.44
1:D:88:ARG:HH22	1:D:138:PHE:HA	1.81	0.44
1:D:198:LEU:O	1:D:201:PHE:N	2.51	0.44
1:F:105:LEU:HG	1:F:105:LEU:H	1.54	0.44
1:G:134:PHE:HZ	1:G:198:LEU:HD23	1.81	0.44
1:B:90:LEU:CD1	1:B:91:THR:N	2.72	0.44
1:C:93:MET:O	1:C:98:MET:HE2	2.17	0.44
1:C:123:ILE:N	1:C:123:ILE:HD13	2.33	0.44
1:D:166:LEU:N	1:D:167:PRO:HD3	2.33	0.44
1:E:132:ALA:CB	1:E:198:LEU:HD21	2.47	0.44
1:F:132:ALA:O	1:F:133:ASN:OD1	2.35	0.44
1:G:177:ALA:O	1:G:180:VAL:HB	2.18	0.44
1:H:147:LEU:HD23	1:H:147:LEU:C	2.38	0.44
1:A:172:GLU:C	1:A:174:VAL:N	2.71	0.43
1:C:128:ILE:CG2	1:C:129:ILE:N	2.81	0.43
1:E:134:PHE:HZ	1:E:198:LEU:HD23	1.81	0.43
1:D:128:ILE:CG2	1:D:129:ILE:N	2.81	0.43
1:E:93:MET:O	1:E:98:MET:HE2	2.17	0.43
1:H:177:ALA:O	1:H:180:VAL:HB	2.18	0.43
1:C:134:PHE:HZ	1:C:198:LEU:HD23	1.83	0.43
1:D:135:SER:HB3	1:D:145:ILE:HD11	2.00	0.43
1:E:93:MET:HA	1:E:97:GLU:OE1	2.18	0.43
1:B:166:LEU:N	1:B:167:PRO:HD3	2.34	0.43
1:G:132:ALA:O	1:G:133:ASN:OD1	2.37	0.43
1:G:166:LEU:N	1:G:167:PRO:HD3	2.33	0.43
1:B:105:LEU:HG	1:B:105:LEU:H	1.55	0.43
1:C:129:ILE:HD12	1:C:193:ARG:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:VAL:O	1:C:175:LYS:C	2.57	0.43
1:E:108:LYS:CD	1:E:121:GLN:HB2	2.49	0.43
1:H:90:LEU:CD1	1:H:91:THR:N	2.73	0.43
1:A:116:CYS:HB3	1:A:118:ARG:HH12	1.84	0.43
1:C:106:ILE:HD12	1:C:122:ALA:CA	2.48	0.43
1:E:105:LEU:HD12	1:E:122:ALA:HB3	2.01	0.43
1:E:179:GLY:CA	1:E:182:ILE:HD12	2.46	0.43
1:F:129:ILE:HD12	1:F:193:ARG:C	2.39	0.43
1:F:172:GLU:C	1:F:174:VAL:N	2.69	0.43
1:H:132:ALA:O	1:H:133:ASN:OD1	2.36	0.43
1:B:106:ILE:HD12	1:B:122:ALA:CA	2.48	0.43
1:D:196:GLU:O	1:D:197:THR:C	2.57	0.43
1:F:108:LYS:HE2	1:F:108:LYS:HB3	1.83	0.43
1:G:135:SER:HB3	1:G:145:ILE:HD11	2.00	0.43
1:H:129:ILE:HD12	1:H:193:ARG:C	2.39	0.43
1:A:151:THR:CG2	1:A:155:ALA:HB3	2.49	0.43
1:C:147:LEU:HD23	1:C:147:LEU:C	2.39	0.43
1:C:196:GLU:O	1:C:197:THR:C	2.56	0.43
1:G:165:SER:C	1:G:167:PRO:HD3	2.38	0.43
1:F:106:ILE:HD12	1:F:122:ALA:CA	2.48	0.43
1:A:98:MET:CE	1:A:133:ASN:ND2	2.82	0.43
1:D:177:ALA:O	1:D:180:VAL:HB	2.19	0.43
1:G:102:TRP:CE3	1:G:156:ILE:HG22	2.54	0.43
1:G:199:GLN:O	1:G:200:ARG:C	2.57	0.43
1:H:93:MET:HA	1:H:97:GLU:OE1	2.19	0.42
1:H:201:PHE:HD1	1:H:201:PHE:HA	1.65	0.42
1:E:92:ASP:N	1:E:133:ASN:OD1	2.45	0.42
1:F:166:LEU:N	1:F:167:PRO:HD3	2.34	0.42
1:D:187:TRP:HH2	1:G:108:LYS:HB3	1.73	0.42
1:F:198:LEU:O	1:F:201:PHE:N	2.52	0.42
1:G:91:THR:CB	1:G:133:ASN:ND2	2.81	0.42
1:G:105:LEU:HG	1:G:105:LEU:H	1.55	0.42
1:G:147:LEU:C	1:G:147:LEU:HD23	2.40	0.42
1:A:166:LEU:N	1:A:167:PRO:HD3	2.34	0.42
1:G:93:MET:HA	1:G:97:GLU:OE1	2.19	0.42
1:A:108:LYS:CD	1:A:121:GLN:HB2	2.50	0.42
1:C:165:SER:OG	1:C:167:PRO:HD3	2.19	0.42
1:E:132:ALA:HB2	1:E:147:LEU:HD12	2.01	0.42
1:G:132:ALA:CB	1:G:198:LEU:HD21	2.50	0.42
1:H:88:ARG:O	1:H:89:TYR:HB2	2.20	0.42
1:B:114:PRO:C	1:B:163:LEU:HG	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:MET:CE	1:C:133:ASN:ND2	2.83	0.42
1:E:174:VAL:O	1:E:175:LYS:C	2.58	0.42
1:B:198:LEU:O	1:B:199:GLN:C	2.58	0.42
1:C:93:MET:HA	1:C:97:GLU:OE1	2.19	0.42
1:E:105:LEU:HG	1:E:105:LEU:H	1.51	0.42
1:F:128:ILE:CG2	1:F:129:ILE:N	2.82	0.42
1:A:132:ALA:O	1:A:133:ASN:OD1	2.37	0.42
1:E:199:GLN:OE1	1:H:105:LEU:HB3	2.19	0.42
1:E:200:ARG:NE	1:H:106:ILE:HD11	2.33	0.42
1:H:108:LYS:CD	1:H:121:GLN:HB2	2.50	0.42
1:D:110:LYS:CE	1:G:187:TRP:O	2.68	0.42
1:G:104:MET:HE3	1:G:104:MET:HB2	1.87	0.42
1:B:138:PHE:CZ	1:C:109:GLN:CG	3.03	0.41
1:F:181:LEU:O	1:F:185:LEU:HG	2.20	0.41
1:G:178:VAL:O	1:G:179:GLY:C	2.58	0.41
1:B:91:THR:CB	1:B:133:ASN:ND2	2.83	0.41
1:B:128:ILE:CG2	1:B:129:ILE:N	2.83	0.41
1:D:133:ASN:O	1:D:144:LEU:HD12	2.20	0.41
1:D:181:LEU:O	1:D:185:LEU:HG	2.20	0.41
1:F:113:GLY:HA3	1:F:114:PRO:HD3	1.84	0.41
1:C:166:LEU:N	1:C:167:PRO:HD3	2.35	0.41
1:C:198:LEU:O	1:C:199:GLN:C	2.59	0.41
1:E:135:SER:HB3	1:E:145:ILE:HD11	2.01	0.41
1:E:196:GLU:O	1:E:197:THR:C	2.58	0.41
1:G:88:ARG:O	1:G:89:TYR:HB2	2.20	0.41
1:H:113:GLY:HA3	1:H:114:PRO:HD3	1.82	0.41
1:B:108:LYS:CD	1:B:121:GLN:HB2	2.50	0.41
1:E:201:PHE:HA	1:E:201:PHE:HD1	1.64	0.41
1:B:108:LYS:HE2	1:B:108:LYS:HB3	1.84	0.41
1:E:165:SER:C	1:E:167:PRO:HD3	2.41	0.41
1:G:128:ILE:CG2	1:G:129:ILE:N	2.83	0.41
1:H:133:ASN:O	1:H:144:LEU:HD12	2.21	0.41
1:D:93:MET:HA	1:D:97:GLU:OE1	2.20	0.41
1:E:98:MET:CE	1:E:133:ASN:ND2	2.84	0.41
1:F:90:LEU:CD1	1:F:91:THR:N	2.76	0.41
1:G:196:GLU:O	1:G:197:THR:C	2.58	0.41
1:H:134:PHE:HZ	1:H:198:LEU:HD23	1.85	0.41
1:H:165:SER:C	1:H:167:PRO:HD3	2.41	0.41
1:C:132:ALA:O	1:C:133:ASN:OD1	2.38	0.41
1:D:132:ALA:HB2	1:D:147:LEU:HB2	2.03	0.41
1:F:132:ALA:HB2	1:F:147:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:NH2	1:B:138:PHE:H	2.17	0.41
1:B:98:MET:SD	1:B:133:ASN:ND2	2.94	0.41
1:B:165:SER:C	1:B:167:PRO:HD3	2.41	0.41
1:D:98:MET:CE	1:D:133:ASN:ND2	2.83	0.41
1:D:116:CYS:HB3	1:D:118:ARG:HH12	1.86	0.41
1:E:198:LEU:O	1:E:199:GLN:C	2.59	0.41
1:G:174:VAL:O	1:G:175:LYS:C	2.59	0.41
1:B:110:LYS:HG2	1:B:111:VAL:N	2.35	0.41
1:A:108:LYS:HB3	1:A:108:LYS:HE2	1.84	0.41
1:A:179:GLY:CA	1:A:182:ILE:HD12	2.49	0.41
1:C:108:LYS:HD2	1:C:121:GLN:HB2	2.02	0.41
1:C:198:LEU:O	1:C:201:PHE:N	2.54	0.41
1:F:198:LEU:O	1:F:199:GLN:C	2.59	0.41
1:H:201:PHE:HA	1:H:202:ALA:HA	1.66	0.41
1:E:114:PRO:C	1:E:163:LEU:HG	2.42	0.41
1:E:153:GLU:OE1	1:E:153:GLU:N	2.51	0.41
1:F:98:MET:SD	1:F:133:ASN:ND2	2.95	0.41
1:E:123:ILE:HD13	1:E:123:ILE:N	2.36	0.40
1:G:106:ILE:HD12	1:G:122:ALA:CA	2.51	0.40
1:G:161:SER:HA	1:G:162:PRO:HD3	1.97	0.40
1:B:133:ASN:O	1:B:144:LEU:HD12	2.21	0.40
1:A:114:PRO:C	1:A:163:LEU:HG	2.41	0.40
1:A:198:LEU:O	1:A:199:GLN:C	2.60	0.40
1:C:181:LEU:O	1:C:185:LEU:HG	2.22	0.40
1:D:110:LYS:HG2	1:D:111:VAL:N	2.36	0.40
1:F:98:MET:CE	1:F:133:ASN:ND2	2.84	0.40
1:H:132:ALA:CB	1:H:198:LEU:HD21	2.49	0.40
1:H:153:GLU:OE1	1:H:153:GLU:N	2.53	0.40
1:B:177:ALA:O	1:B:180:VAL:HB	2.21	0.40
1:D:106:ILE:HD12	1:D:122:ALA:CA	2.51	0.40
1:F:105:LEU:HD12	1:F:122:ALA:HB3	2.03	0.40
1:E:110:LYS:HG2	1:E:111:VAL:N	2.36	0.40
1:E:181:LEU:O	1:E:185:LEU:HG	2.21	0.40
1:F:177:ALA:O	1:F:180:VAL:HB	2.22	0.40
1:H:174:VAL:O	1:H:175:LYS:C	2.60	0.40
1:B:139:ASP:HA	1:A:106:ILE:CD1	2.51	0.40
1:B:174:VAL:O	1:B:175:LYS:C	2.59	0.40
1:A:110:LYS:HG2	1:A:111:VAL:N	2.37	0.40
1:A:143:THR:HG23	1:A:169:HIS:NE2	2.37	0.40
1:C:92:ASP:N	1:C:133:ASN:OD1	2.46	0.40
1:C:201:PHE:HA	1:C:201:PHE:HD1	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:PRO:C	1:F:163:LEU:HG	2.42	0.40
1:G:198:LEU:O	1:G:199:GLN:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	114/152 (75%)	88 (77%)	22 (19%)	4 (4%)	3	24
1	B	114/152 (75%)	89 (78%)	22 (19%)	3 (3%)	5	31
1	C	114/152 (75%)	89 (78%)	22 (19%)	3 (3%)	5	31
1	D	114/152 (75%)	89 (78%)	21 (18%)	4 (4%)	3	24
1	E	114/152 (75%)	88 (77%)	23 (20%)	3 (3%)	5	31
1	F	112/152 (74%)	88 (79%)	22 (20%)	2 (2%)	8	41
1	G	114/152 (75%)	89 (78%)	22 (19%)	3 (3%)	5	31
1	H	114/152 (75%)	87 (76%)	25 (22%)	2 (2%)	8	41
All	All	910/1216 (75%)	707 (78%)	179 (20%)	24 (3%)	5	31

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	TYR
1	D	88	ARG
1	D	89	TYR
1	C	88	ARG
1	E	88	ARG
1	E	174	VAL
1	G	88	ARG
1	B	89	TYR

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Mol	Chain	Res	Type
1	B	174	VAL
1	A	88	ARG
1	A	174	VAL
1	C	176	ASN
1	D	174	VAL
1	F	174	VAL
1	G	176	ASN
1	H	174	VAL
1	H	176	ASN
1	B	176	ASN
1	A	176	ASN
1	C	174	VAL
1	D	176	ASN
1	E	176	ASN
1	F	176	ASN
1	G	174	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	101/132 (76%)	99 (98%)	2 (2%)	55	80
1	B	101/132 (76%)	99 (98%)	2 (2%)	55	80
1	C	101/132 (76%)	99 (98%)	2 (2%)	55	80
1	D	101/132 (76%)	96 (95%)	5 (5%)	24	60
1	E	101/132 (76%)	99 (98%)	2 (2%)	55	80
1	F	99/132 (75%)	96 (97%)	3 (3%)	41	73
1	G	101/132 (76%)	99 (98%)	2 (2%)	55	80
1	H	101/132 (76%)	100 (99%)	1 (1%)	76	90
All	All	806/1056 (76%)	787 (98%)	19 (2%)	49	77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	LEU
1	B	201	PHE
1	A	105	LEU
1	A	201	PHE
1	C	105	LEU
1	C	201	PHE
1	D	87	SER
1	D	88	ARG
1	D	105	LEU
1	D	147	LEU
1	D	201	PHE
1	E	105	LEU
1	E	201	PHE
1	F	105	LEU
1	F	147	LEU
1	F	201	PHE
1	G	105	LEU
1	G	201	PHE
1	H	201	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	116/152 (76%)	-0.46	0	100	100	45, 73, 118, 160	1 (0%)
1	B	116/152 (76%)	-0.43	0	100	100	42, 76, 120, 163	1 (0%)
1	C	116/152 (76%)	-0.50	0	100	100	41, 79, 122, 153	1 (0%)
1	D	116/152 (76%)	-0.50	0	100	100	45, 80, 119, 153	0
1	E	116/152 (76%)	-0.47	0	100	100	47, 80, 126, 156	0
1	F	114/152 (75%)	-0.53	0	100	100	46, 80, 120, 148	0
1	G	116/152 (76%)	-0.50	0	100	100	44, 85, 124, 165	1 (0%)
1	H	116/152 (76%)	-0.50	0	100	100	52, 84, 126, 163	1 (0%)
All	All	926/1216 (76%)	-0.49	0	100	100	41, 80, 123, 165	5 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.