



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:41 PM GMT

PDB ID : 1BVS
Title : RUVA COMPLEXED TO A HOLLIDAY JUNCTION.
Authors : Roe, S.M.; Pearl, L.H.
Deposited on : 1998-09-17
Resolution : 3.00 Å(reported)

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

The following versions of software and data (see [references ⓘ](#)) 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

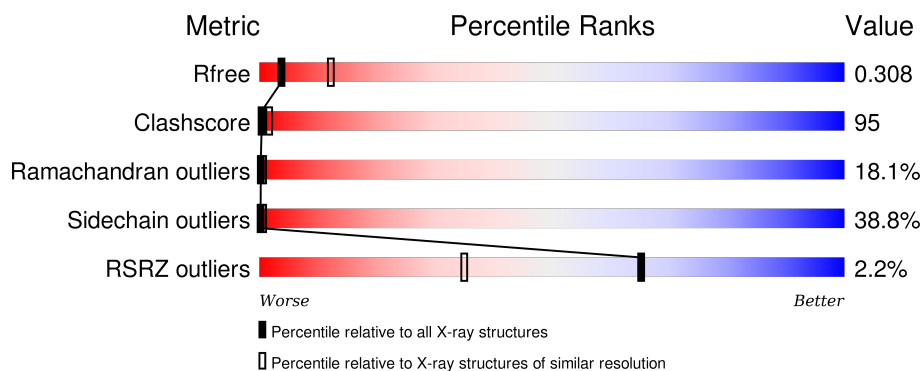
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	<div> <div>4%</div> <div>16%</div> <div>44%</div> <div>28%</div> <div>10%</div> </div>
1	B	203	<div> <div>13%</div> <div>41%</div> <div>32%</div> <div>10%</div> </div>
1	C	203	<div> <div>4%</div> <div>16%</div> <div>44%</div> <div>28%</div> <div>10%</div> </div>
1	D	203	<div> <div>13%</div> <div>41%</div> <div>32%</div> <div>10%</div> </div>
1	E	203	<div> <div>4%</div> <div>16%</div> <div>43%</div> <div>29%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	203	<div><div></div><div>13%41%32%•10%</div></div>
1	G	203	<div><div>2%</div><div>16%43%29%•10%</div></div>
1	H	203	<div><div></div><div>13%40%33%•10%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10448 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 PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1303	815	233	251	4			
1	B	183	Total	C	N	O	S	0	0	0
			1309	815	234	256	4			
1	C	183	Total	C	N	O	S	0	0	0
			1303	815	233	251	4			
1	D	183	Total	C	N	O	S	0	0	0
			1309	815	234	256	4			
1	E	183	Total	C	N	O	S	0	0	0
			1303	815	233	251	4			
1	F	183	Total	C	N	O	S	0	0	0
			1309	815	234	256	4			
1	G	183	Total	C	N	O	S	0	0	0
			1303	815	233	251	4			
1	H	183	Total	C	N	O	S	0	0	0
			1309	815	234	256	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ASN	ARG	CONFLICT	UNP P40832
A	117	ARG	LYS	CONFLICT	UNP P40832
B	39	ASN	ARG	CONFLICT	UNP P40832
B	117	ARG	LYS	CONFLICT	UNP P40832
C	39	ASN	ARG	CONFLICT	UNP P40832
C	117	ARG	LYS	CONFLICT	UNP P40832
D	39	ASN	ARG	CONFLICT	UNP P40832
D	117	ARG	LYS	CONFLICT	UNP P40832
E	39	ASN	ARG	CONFLICT	UNP P40832
E	117	ARG	LYS	CONFLICT	UNP P40832
F	39	ASN	ARG	CONFLICT	UNP P40832
F	117	ARG	LYS	CONFLICT	UNP P40832
G	39	ASN	ARG	CONFLICT	UNP P40832

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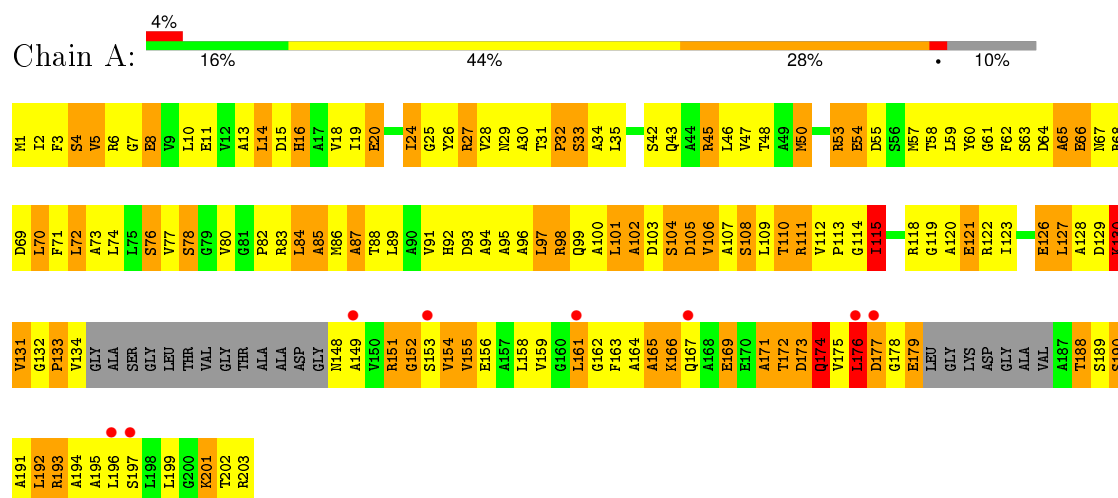
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Chain	Residue	Modelled	Actual	Comment	Reference
G	117	ARG	LYS	CONFLICT	UNP P40832
H	39	ASN	ARG	CONFLICT	UNP P40832
H	117	ARG	LYS	CONFLICT	UNP P40832

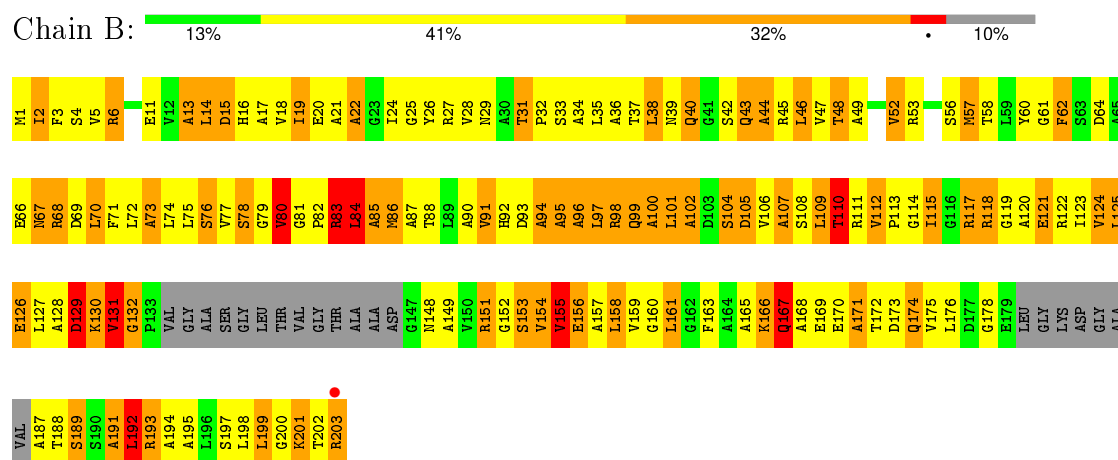
3 Residue-property plots

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.

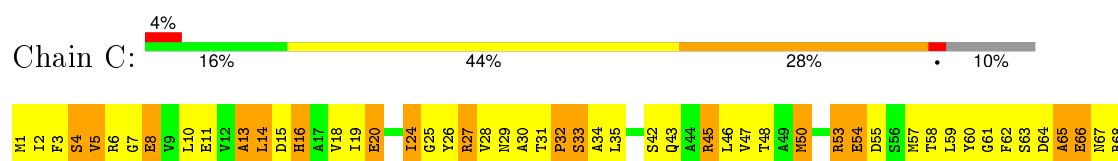
• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)

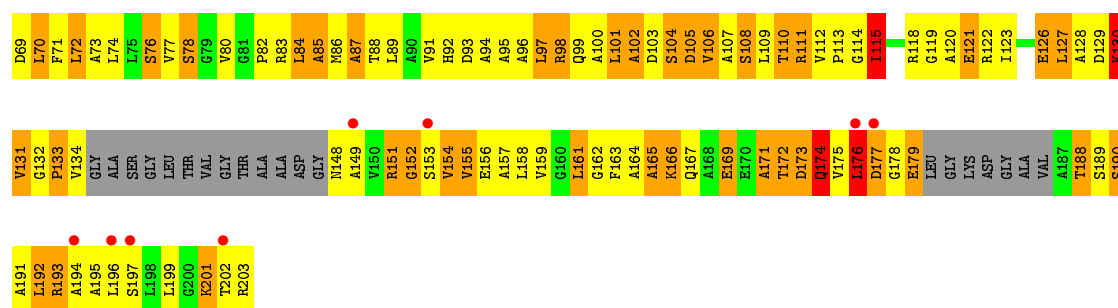


• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)



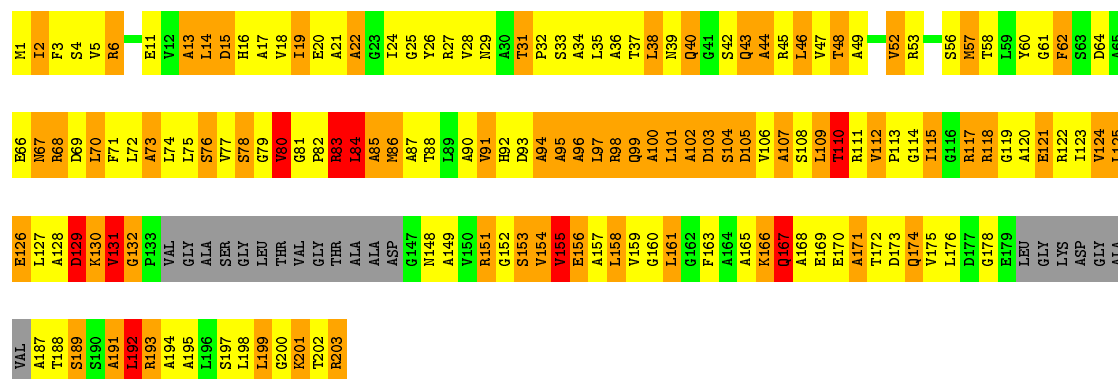
• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)





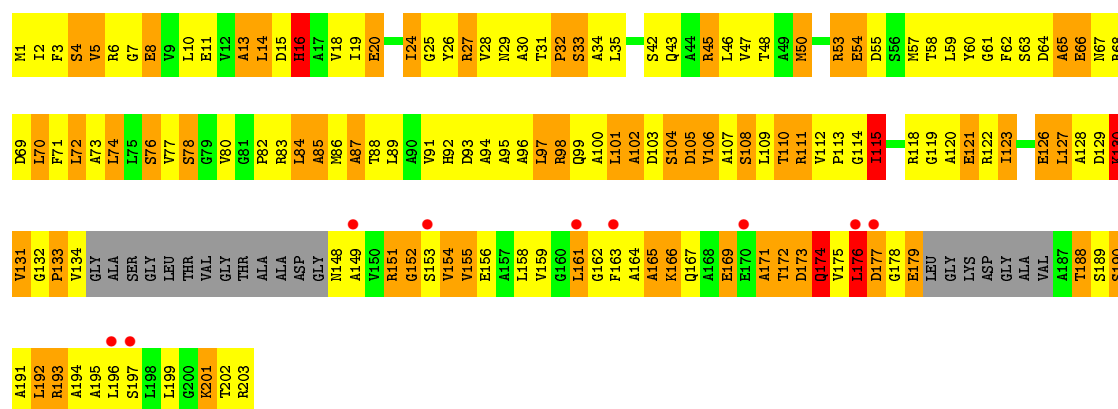
• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)

Chain D: 13% 41% 32% 10%



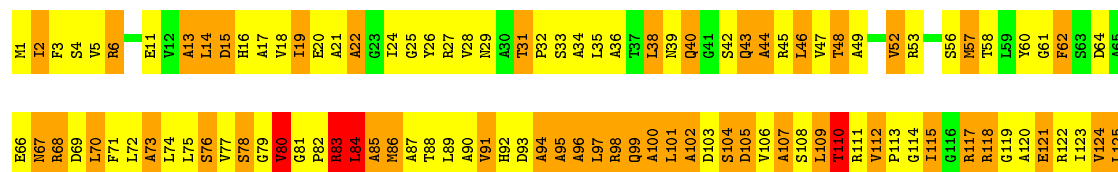
• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)

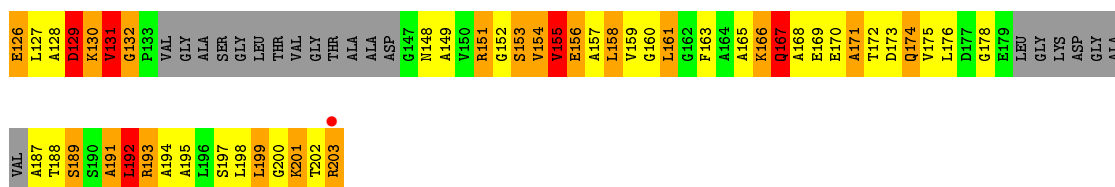
Chain E: 4% 16% 43% 29% 10%



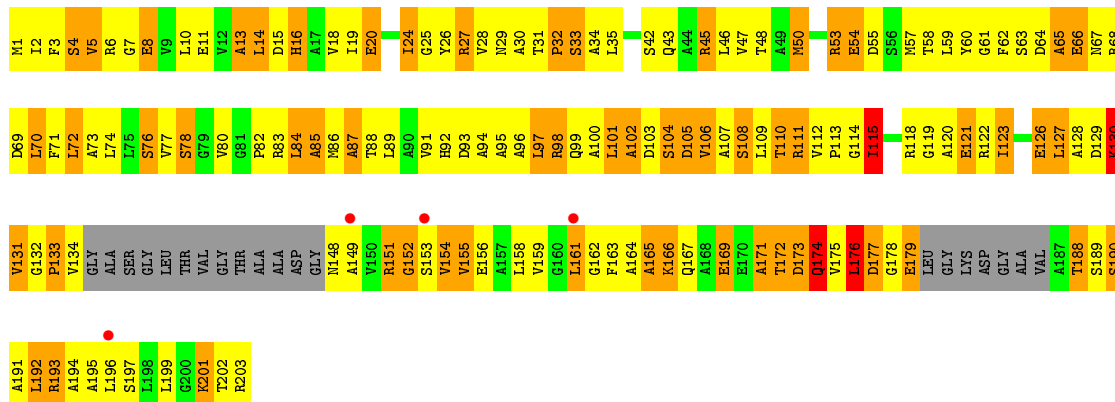
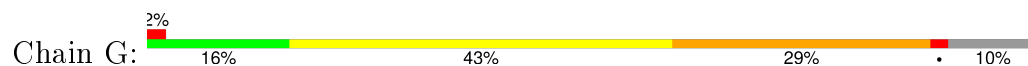
• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)

Chain F: 13% 41% 32% 10%

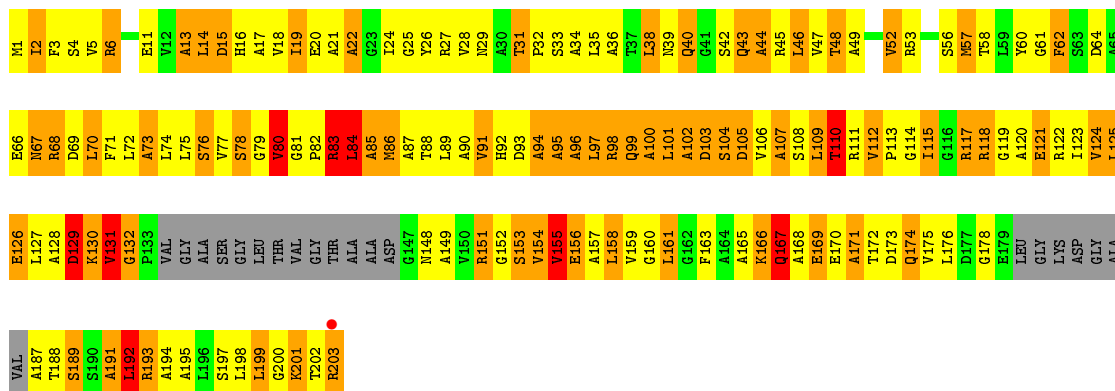




• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)



• Molecule 1: PROTEIN (HOLLIDAY JUNCTION DNA HELICASE RUVA)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	142.63Å 142.63Å 108.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 36.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.00) 99.9 (36.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 3.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.274 , 0.319 0.266 , 0.308	Depositor DCC
R_{free} test set	2490 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.477 for -h,-k,l 0.478 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 49147 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	0/1312	0.89	2/1779 (0.1%)
1	B	0.63	0/1318	0.92	0/1786
1	C	0.65	0/1312	0.89	3/1779 (0.2%)
1	D	0.63	0/1318	0.92	0/1786
1	E	0.65	0/1312	0.89	3/1779 (0.2%)
1	F	0.64	0/1318	0.92	0/1786
1	G	0.64	0/1312	0.89	3/1779 (0.2%)
1	H	0.63	0/1318	0.92	0/1786
All	All	0.64	0/10520	0.90	11/14260 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	132	GLY	N-CA-C	-7.20	95.09	113.10
1	A	132	GLY	N-CA-C	-7.20	95.11	113.10
1	E	132	GLY	N-CA-C	-7.17	95.17	113.10
1	C	132	GLY	N-CA-C	-7.17	95.19	113.10
1	E	127	LEU	CA-CB-CG	-6.21	101.02	115.30
1	A	127	LEU	CA-CB-CG	-6.10	101.27	115.30
1	C	127	LEU	CA-CB-CG	-6.04	101.40	115.30
1	G	127	LEU	CA-CB-CG	-5.98	101.55	115.30
1	E	13	ALA	N-CA-C	-5.04	97.40	111.00
1	C	13	ALA	N-CA-C	-5.03	97.42	111.00
1	G	13	ALA	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1303	0	1331	251	0
1	B	1309	0	1333	257	0
1	C	1303	0	1331	255	0
1	D	1309	0	1333	258	0
1	E	1303	0	1331	249	0
1	F	1309	0	1333	263	0
1	G	1303	0	1331	253	0
1	H	1309	0	1333	259	0
All	All	10448	0	10656	1996	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 95.

All (1996) 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:D:2:ILE:HG22	1:D:48:THR:HG21	1.16	1.15
1:B:2:ILE:HG22	1:B:48:THR:HG21	1.15	1.15
1:D:84:LEU:HD12	1:D:84:LEU:H	1.15	1.11
1:F:84:LEU:H	1:F:84:LEU:HD12	1.16	1.11
1:F:2:ILE:HG22	1:F:48:THR:HG21	1.16	1.10
1:H:84:LEU:HD12	1:H:84:LEU:H	1.15	1.10
1:A:91:VAL:HG12	1:A:92:HIS:CD2	1.87	1.10
1:B:84:LEU:HD12	1:B:84:LEU:H	1.14	1.09
1:G:91:VAL:HG12	1:G:92:HIS:CD2	1.88	1.09
1:F:91:VAL:HG12	1:F:92:HIS:H	1.12	1.09
1:C:91:VAL:HG12	1:C:92:HIS:CD2	1.87	1.08
1:H:2:ILE:HG22	1:H:48:THR:HG21	1.15	1.08
1:E:91:VAL:HG12	1:E:92:HIS:CD2	1.88	1.08
1:D:91:VAL:HG12	1:D:92:HIS:H	1.11	1.07
1:B:91:VAL:HG12	1:B:92:HIS:H	1.12	1.07
1:H:91:VAL:HG12	1:H:92:HIS:H	1.12	1.06
1:A:4:SER:O	1:A:5:VAL:HG23	1.57	1.04
1:E:4:SER:O	1:E:5:VAL:HG23	1.58	1.04
1:E:129:ASP:O	1:E:133:PRO:HD2	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:SER:O	1:G:5:VAL:HG23	1.57	1.03
1:C:129:ASP:O	1:C:133:PRO:HD2	1.59	1.02
1:C:4:SER:O	1:C:5:VAL:HG23	1.58	1.02
1:A:129:ASP:O	1:A:133:PRO:HD2	1.58	1.02
1:G:129:ASP:O	1:G:133:PRO:HD2	1.59	1.01
1:E:46:LEU:O	1:E:48:THR:HG23	1.61	1.01
1:A:46:LEU:O	1:A:48:THR:HG23	1.60	1.00
1:D:27:ARG:HH11	1:D:29:ASN:HD21	1.06	1.00
1:G:46:LEU:O	1:G:48:THR:HG23	1.61	1.00
1:H:83:ARG:HB2	1:H:84:LEU:HD12	1.42	0.99
1:B:27:ARG:HH11	1:B:29:ASN:HD21	1.06	0.98
1:D:83:ARG:HB2	1:D:84:LEU:HD12	1.41	0.98
1:C:46:LEU:O	1:C:48:THR:HG23	1.61	0.98
1:B:83:ARG:HB2	1:B:84:LEU:HD12	1.41	0.97
1:F:83:ARG:HB2	1:F:84:LEU:HD12	1.41	0.97
1:A:91:VAL:HG12	1:A:92:HIS:HD2	1.28	0.95
1:H:14:LEU:HD12	1:H:14:LEU:H	1.29	0.95
1:F:27:ARG:HH11	1:F:29:ASN:HD21	1.07	0.94
1:B:14:LEU:HD12	1:B:14:LEU:H	1.31	0.94
1:D:14:LEU:H	1:D:14:LEU:HD12	1.31	0.94
1:H:91:VAL:HG12	1:H:92:HIS:N	1.82	0.94
1:F:14:LEU:HD12	1:F:14:LEU:H	1.31	0.93
1:D:91:VAL:HG12	1:D:92:HIS:N	1.82	0.93
1:F:91:VAL:HG12	1:F:92:HIS:N	1.82	0.93
1:C:91:VAL:HG12	1:C:92:HIS:HD2	1.28	0.93
1:H:130:LYS:O	1:H:131:VAL:HB	1.70	0.92
1:H:27:ARG:HH11	1:H:29:ASN:HD21	1.06	0.92
1:F:70:LEU:O	1:F:74:LEU:HD12	1.69	0.92
1:B:84:LEU:HD12	1:B:84:LEU:N	1.84	0.92
1:B:84:LEU:H	1:B:84:LEU:CD1	1.83	0.92
1:H:191:ALA:O	1:H:194:ALA:N	2.02	0.92
1:D:191:ALA:O	1:D:194:ALA:N	2.03	0.91
1:D:70:LEU:O	1:D:74:LEU:HD12	1.69	0.91
1:B:70:LEU:O	1:B:74:LEU:HD12	1.69	0.91
1:G:91:VAL:HG12	1:G:92:HIS:HD2	1.28	0.91
1:D:84:LEU:CD1	1:D:84:LEU:H	1.84	0.91
1:A:193:ARG:HA	1:A:196:LEU:HG	1.53	0.91
1:B:191:ALA:O	1:B:194:ALA:N	2.03	0.91
1:F:130:LYS:O	1:F:131:VAL:HB	1.70	0.90
1:F:191:ALA:O	1:F:194:ALA:N	2.02	0.90
1:E:193:ARG:HA	1:E:196:LEU:HG	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:HA	1:A:176:LEU:HD23	1.54	0.90
1:H:84:LEU:HD12	1:H:84:LEU:N	1.86	0.90
1:D:84:LEU:HD12	1:D:84:LEU:N	1.85	0.90
1:H:84:LEU:CD1	1:H:84:LEU:H	1.84	0.90
1:F:84:LEU:N	1:F:84:LEU:HD12	1.85	0.90
1:B:91:VAL:HG12	1:B:92:HIS:N	1.82	0.90
1:C:153:SER:HA	1:C:156:GLU:HB2	1.53	0.90
1:C:193:ARG:HA	1:C:196:LEU:HG	1.54	0.90
1:B:130:LYS:O	1:B:131:VAL:HB	1.70	0.90
1:H:27:ARG:HH11	1:H:29:ASN:ND2	1.69	0.90
1:H:70:LEU:O	1:H:74:LEU:HD12	1.70	0.90
1:D:27:ARG:HH11	1:D:29:ASN:ND2	1.69	0.90
1:G:173:ASP:HA	1:G:176:LEU:HD23	1.54	0.90
1:F:84:LEU:H	1:F:84:LEU:CD1	1.84	0.89
1:E:91:VAL:HG12	1:E:92:HIS:HD2	1.27	0.89
1:G:153:SER:HA	1:G:156:GLU:HB2	1.54	0.89
1:F:27:ARG:HH11	1:F:29:ASN:ND2	1.69	0.89
1:G:20:GLU:HA	1:G:25:GLY:HA2	1.55	0.89
1:C:20:GLU:HA	1:C:25:GLY:HA2	1.55	0.89
1:H:2:ILE:CG2	1:H:48:THR:HG21	2.02	0.89
1:E:20:GLU:HA	1:E:25:GLY:HA2	1.54	0.89
1:G:112:VAL:O	1:G:115:ILE:HB	1.72	0.89
1:E:112:VAL:O	1:E:115:ILE:HB	1.73	0.89
1:B:27:ARG:HH11	1:B:29:ASN:ND2	1.68	0.89
1:D:130:LYS:O	1:D:131:VAL:HB	1.70	0.88
1:G:193:ARG:HA	1:G:196:LEU:HG	1.53	0.88
1:C:173:ASP:HA	1:C:176:LEU:HD23	1.54	0.88
1:B:161:LEU:HD23	1:B:161:LEU:N	1.88	0.88
1:A:20:GLU:HA	1:A:25:GLY:HA2	1.55	0.88
1:F:2:ILE:CG2	1:F:48:THR:HG21	2.03	0.88
1:F:161:LEU:HD23	1:F:161:LEU:N	1.88	0.88
1:A:112:VAL:O	1:A:115:ILE:HB	1.72	0.88
1:B:195:ALA:O	1:B:199:LEU:HD12	1.74	0.88
1:E:173:ASP:HA	1:E:176:LEU:HD23	1.53	0.88
1:A:153:SER:HA	1:A:156:GLU:HB2	1.54	0.88
1:C:112:VAL:O	1:C:115:ILE:HB	1.73	0.88
1:E:153:SER:HA	1:E:156:GLU:HB2	1.54	0.87
1:D:161:LEU:HD23	1:D:161:LEU:N	1.89	0.87
1:H:161:LEU:N	1:H:161:LEU:HD23	1.89	0.87
1:D:2:ILE:CG2	1:D:48:THR:HG21	2.03	0.87
1:H:195:ALA:O	1:H:199:LEU:HD12	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:ALA:O	1:F:199:LEU:HD12	1.73	0.86
1:H:155:VAL:O	1:H:159:VAL:HG23	1.75	0.86
1:D:155:VAL:O	1:D:159:VAL:HG23	1.75	0.86
1:B:2:ILE:CG2	1:B:48:THR:HG21	2.03	0.86
1:G:153:SER:C	1:G:155:VAL:H	1.80	0.85
1:F:155:VAL:O	1:F:159:VAL:HG23	1.75	0.85
1:B:155:VAL:O	1:B:159:VAL:HG23	1.75	0.85
1:D:195:ALA:O	1:D:199:LEU:HD12	1.75	0.85
1:D:91:VAL:CG1	1:D:92:HIS:H	1.89	0.85
1:A:172:THR:HG23	1:A:173:ASP:H	1.42	0.84
1:G:172:THR:HG23	1:G:173:ASP:H	1.43	0.84
1:E:172:THR:HG23	1:E:173:ASP:H	1.42	0.84
1:H:77:VAL:HG12	1:H:78:SER:N	1.92	0.84
1:G:54:GLU:OE1	1:G:55:ASP:HB3	1.77	0.84
1:A:54:GLU:OE1	1:A:55:ASP:HB3	1.77	0.84
1:C:54:GLU:OE1	1:C:55:ASP:HB3	1.78	0.84
1:C:193:ARG:HA	1:C:196:LEU:CG	2.08	0.84
1:B:198:LEU:O	1:B:200:GLY:N	2.10	0.84
1:F:77:VAL:HG12	1:F:78:SER:N	1.92	0.83
1:A:153:SER:C	1:A:155:VAL:H	1.80	0.83
1:D:77:VAL:HG12	1:D:78:SER:N	1.92	0.83
1:E:193:ARG:HA	1:E:196:LEU:CG	2.08	0.83
1:C:153:SER:C	1:C:155:VAL:H	1.80	0.83
1:G:193:ARG:HA	1:G:196:LEU:CG	2.08	0.82
1:H:70:LEU:HD23	1:H:70:LEU:N	1.95	0.82
1:A:193:ARG:HA	1:A:196:LEU:CG	2.08	0.82
1:H:198:LEU:O	1:H:200:GLY:N	2.12	0.82
1:C:172:THR:HG23	1:C:173:ASP:H	1.43	0.82
1:E:6:ARG:HG3	1:E:45:ARG:HB2	1.62	0.82
1:E:54:GLU:OE1	1:E:55:ASP:HB3	1.79	0.82
1:G:4:SER:HB2	1:G:45:ARG:HD2	1.62	0.82
1:A:4:SER:HB2	1:A:45:ARG:HD2	1.62	0.81
1:B:70:LEU:HD23	1:B:70:LEU:N	1.95	0.81
1:B:77:VAL:HG12	1:B:78:SER:N	1.93	0.81
1:A:6:ARG:HG3	1:A:45:ARG:HB2	1.62	0.81
1:E:153:SER:C	1:E:155:VAL:H	1.80	0.81
1:C:4:SER:HB2	1:C:45:ARG:HD2	1.63	0.81
1:D:198:LEU:O	1:D:200:GLY:N	2.13	0.81
1:B:161:LEU:HD23	1:B:161:LEU:H	1.46	0.81
1:D:161:LEU:HD23	1:D:161:LEU:H	1.45	0.81
1:F:198:LEU:O	1:F:200:GLY:N	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:LEU:HD23	1:F:70:LEU:N	1.94	0.81
1:A:179:GLU:HG3	1:A:179:GLU:O	1.81	0.81
1:F:31:THR:HG22	1:F:86:MET:HE1	1.62	0.81
1:B:31:THR:HG22	1:B:86:MET:CE	2.11	0.80
1:C:5:VAL:HG12	1:C:5:VAL:O	1.81	0.80
1:F:161:LEU:HD23	1:F:161:LEU:H	1.46	0.80
1:H:31:THR:HG22	1:H:86:MET:CE	2.11	0.80
1:E:4:SER:HB2	1:E:45:ARG:HD2	1.63	0.80
1:D:31:THR:HG22	1:D:86:MET:CE	2.12	0.80
1:G:6:ARG:HG3	1:G:45:ARG:HB2	1.62	0.80
1:E:57:MET:O	1:F:1:MET:HB2	1.82	0.80
1:D:70:LEU:N	1:D:70:LEU:HD23	1.96	0.79
1:F:70:LEU:HD23	1:F:70:LEU:H	1.45	0.79
1:C:115:ILE:HG22	1:C:115:ILE:O	1.82	0.79
1:B:70:LEU:HD23	1:B:70:LEU:H	1.46	0.79
1:C:158:LEU:HD22	1:C:158:LEU:H	1.47	0.79
1:C:179:GLU:O	1:C:179:GLU:HG3	1.81	0.79
1:C:57:MET:O	1:D:1:MET:HB2	1.83	0.79
1:A:115:ILE:O	1:A:115:ILE:HG22	1.82	0.79
1:G:115:ILE:O	1:G:115:ILE:HG22	1.81	0.79
1:H:70:LEU:HD23	1:H:70:LEU:H	1.45	0.79
1:E:5:VAL:O	1:E:5:VAL:HG12	1.82	0.79
1:B:109:LEU:O	1:B:111:ARG:N	2.16	0.79
1:G:5:VAL:O	1:G:5:VAL:HG12	1.81	0.79
1:F:31:THR:HG22	1:F:86:MET:CE	2.13	0.79
1:E:115:ILE:O	1:E:115:ILE:HG22	1.83	0.79
1:D:109:LEU:O	1:D:111:ARG:N	2.16	0.79
1:C:6:ARG:HG3	1:C:45:ARG:HB2	1.62	0.79
1:F:109:LEU:O	1:F:111:ARG:N	2.15	0.78
1:A:6:ARG:HA	1:A:45:ARG:HA	1.65	0.78
1:C:6:ARG:HA	1:C:45:ARG:HA	1.64	0.78
1:B:70:LEU:O	1:B:73:ALA:HB3	1.83	0.78
1:A:5:VAL:HG12	1:A:5:VAL:O	1.82	0.78
1:H:109:LEU:O	1:H:111:ARG:N	2.17	0.78
1:G:179:GLU:HG3	1:G:179:GLU:O	1.82	0.78
1:E:155:VAL:HA	1:E:158:LEU:HD23	1.66	0.78
1:E:158:LEU:H	1:E:158:LEU:HD22	1.49	0.78
1:A:57:MET:O	1:B:1:MET:HB2	1.84	0.78
1:E:179:GLU:HG3	1:E:179:GLU:O	1.81	0.78
1:E:6:ARG:HA	1:E:45:ARG:HA	1.64	0.78
1:G:155:VAL:HA	1:G:158:LEU:HD23	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:VAL:HA	1:C:158:LEU:HD23	1.66	0.77
1:A:163:PHE:HE1	1:D:112:VAL:HA	1.50	0.77
1:G:57:MET:O	1:H:1:MET:HB2	1.84	0.77
1:D:70:LEU:O	1:D:73:ALA:HB3	1.84	0.77
1:B:3:PHE:HA	1:B:48:THR:HG22	1.67	0.77
1:G:158:LEU:HD22	1:G:158:LEU:H	1.49	0.77
1:H:161:LEU:HD23	1:H:161:LEU:H	1.47	0.77
1:G:6:ARG:HA	1:G:45:ARG:HA	1.65	0.77
1:H:77:VAL:HG12	1:H:78:SER:H	1.50	0.77
1:D:3:PHE:HA	1:D:48:THR:HG22	1.66	0.77
1:H:70:LEU:O	1:H:73:ALA:HB3	1.85	0.77
1:F:70:LEU:O	1:F:73:ALA:HB3	1.85	0.77
1:G:126:GLU:HA	1:G:126:GLU:OE1	1.85	0.76
1:A:158:LEU:HD22	1:A:158:LEU:H	1.49	0.76
1:D:77:VAL:HG12	1:D:78:SER:H	1.49	0.76
1:H:80:VAL:O	1:H:84:LEU:HD13	1.86	0.76
1:A:155:VAL:HA	1:A:158:LEU:HD23	1.67	0.76
1:D:70:LEU:HD23	1:D:70:LEU:H	1.47	0.76
1:E:126:GLU:OE1	1:E:126:GLU:HA	1.86	0.76
1:H:52:VAL:O	1:H:53:ARG:HD3	1.85	0.76
1:B:48:THR:HG23	1:B:49:ALA:N	2.01	0.75
1:F:77:VAL:HG12	1:F:78:SER:H	1.50	0.75
1:A:126:GLU:OE1	1:A:126:GLU:HA	1.86	0.75
1:B:189:SER:HB2	1:B:193:ARG:HH12	1.51	0.75
1:B:27:ARG:NH1	1:B:29:ASN:HD21	1.83	0.75
1:B:80:VAL:O	1:B:84:LEU:HD13	1.87	0.75
1:F:3:PHE:HA	1:F:48:THR:HG22	1.67	0.75
1:H:2:ILE:HG22	1:H:48:THR:CG2	2.08	0.75
1:D:31:THR:HG22	1:D:86:MET:HE1	1.69	0.75
1:H:48:THR:HG23	1:H:49:ALA:N	2.01	0.75
1:B:110:THR:HA	1:B:115:ILE:HG22	1.68	0.75
1:D:80:VAL:O	1:D:84:LEU:HD13	1.86	0.75
1:H:3:PHE:HA	1:H:48:THR:HG22	1.67	0.75
1:C:126:GLU:OE1	1:C:126:GLU:HA	1.86	0.75
1:D:95:ALA:O	1:D:97:LEU:N	2.19	0.75
1:H:110:THR:HA	1:H:115:ILE:HG22	1.68	0.75
1:F:155:VAL:HG12	1:F:156:GLU:N	2.02	0.75
1:F:52:VAL:O	1:F:53:ARG:HD3	1.87	0.74
1:F:110:THR:HA	1:F:115:ILE:HG22	1.68	0.74
1:B:77:VAL:HG12	1:B:78:SER:H	1.50	0.74
1:F:95:ALA:O	1:F:97:LEU:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:SER:HB2	1:F:193:ARG:HH12	1.51	0.74
1:H:95:ALA:O	1:H:97:LEU:N	2.20	0.74
1:C:101:LEU:HD22	1:C:101:LEU:H	1.51	0.74
1:F:112:VAL:HA	1:G:163:PHE:HE1	1.52	0.74
1:B:99:GLN:O	1:B:100:ALA:C	2.26	0.74
1:G:101:LEU:HD22	1:G:101:LEU:H	1.52	0.74
1:B:95:ALA:O	1:B:97:LEU:N	2.20	0.74
1:H:99:GLN:O	1:H:100:ALA:C	2.26	0.74
1:D:48:THR:HG23	1:D:49:ALA:N	2.01	0.73
1:F:80:VAL:O	1:F:84:LEU:HD13	1.87	0.73
1:E:163:PHE:HE1	1:H:112:VAL:HA	1.52	0.73
1:D:27:ARG:NH1	1:D:29:ASN:HD21	1.84	0.73
1:F:99:GLN:O	1:F:100:ALA:C	2.26	0.73
1:B:13:ALA:HB3	1:B:16:HIS:O	1.88	0.73
1:H:31:THR:HG22	1:H:86:MET:HE1	1.68	0.73
1:H:13:ALA:HB3	1:H:16:HIS:O	1.88	0.73
1:C:13:ALA:HB3	1:C:16:HIS:CD2	2.24	0.73
1:H:167:GLN:HE21	1:H:167:GLN:HA	1.54	0.73
1:F:3:PHE:C	1:F:48:THR:HB	2.09	0.73
1:H:189:SER:HB2	1:H:193:ARG:HH12	1.52	0.73
1:D:167:GLN:HA	1:D:167:GLN:HE21	1.53	0.73
1:D:52:VAL:O	1:D:53:ARG:HD3	1.88	0.73
1:D:189:SER:HB2	1:D:193:ARG:HH12	1.53	0.73
1:F:167:GLN:HA	1:F:167:GLN:HE21	1.53	0.73
1:F:6:ARG:HA	1:F:45:ARG:HA	1.71	0.73
1:C:13:ALA:HB3	1:C:16:HIS:HD2	1.54	0.73
1:F:48:THR:HG23	1:F:49:ALA:N	2.03	0.73
1:C:70:LEU:O	1:C:73:ALA:HB3	1.88	0.73
1:H:6:ARG:HA	1:H:45:ARG:HA	1.71	0.73
1:H:27:ARG:NH1	1:H:29:ASN:HD21	1.84	0.73
1:B:167:GLN:HE21	1:B:167:GLN:HA	1.53	0.73
1:E:101:LEU:HD22	1:E:101:LEU:H	1.54	0.73
1:B:52:VAL:O	1:B:53:ARG:HD3	1.87	0.73
1:D:2:ILE:HG22	1:D:48:THR:CG2	2.09	0.73
1:E:13:ALA:HB3	1:E:16:HIS:HD2	1.54	0.73
1:B:194:ALA:O	1:B:197:SER:HB3	1.88	0.73
1:F:2:ILE:HG22	1:F:48:THR:CG2	2.08	0.72
1:H:3:PHE:C	1:H:48:THR:HB	2.09	0.72
1:D:6:ARG:HA	1:D:45:ARG:HA	1.70	0.72
1:D:110:THR:HA	1:D:115:ILE:HG22	1.69	0.72
1:A:70:LEU:O	1:A:73:ALA:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LEU:HG	1:C:177:ASP:H	1.55	0.72
1:B:6:ARG:HA	1:B:45:ARG:HA	1.69	0.72
1:B:2:ILE:HG22	1:B:48:THR:CG2	2.08	0.72
1:G:176:LEU:HG	1:G:177:ASP:H	1.54	0.72
1:F:27:ARG:NH1	1:F:29:ASN:HD21	1.84	0.72
1:A:73:ALA:O	1:A:76:SER:HB3	1.90	0.72
1:C:73:ALA:O	1:C:76:SER:HB3	1.89	0.72
1:A:176:LEU:HG	1:A:177:ASP:H	1.55	0.72
1:G:13:ALA:HB3	1:G:16:HIS:CD2	2.25	0.72
1:E:176:LEU:HG	1:E:177:ASP:H	1.55	0.72
1:E:70:LEU:O	1:E:73:ALA:HB3	1.88	0.72
1:G:77:VAL:HG12	1:G:78:SER:N	2.05	0.72
1:C:66:GLU:O	1:C:70:LEU:HD13	1.89	0.72
1:B:3:PHE:C	1:B:48:THR:HB	2.09	0.72
1:D:99:GLN:O	1:D:100:ALA:C	2.27	0.72
1:A:13:ALA:HB3	1:A:16:HIS:CD2	2.25	0.72
1:G:13:ALA:HB3	1:G:16:HIS:HD2	1.55	0.72
1:E:73:ALA:O	1:E:76:SER:HB3	1.89	0.72
1:A:101:LEU:HD22	1:A:101:LEU:H	1.55	0.72
1:B:112:VAL:HA	1:C:163:PHE:HE1	1.53	0.72
1:D:155:VAL:HG12	1:D:156:GLU:N	2.03	0.72
1:A:77:VAL:HG12	1:A:78:SER:N	2.05	0.71
1:H:194:ALA:O	1:H:197:SER:HB3	1.88	0.71
1:F:194:ALA:O	1:F:197:SER:HB3	1.90	0.71
1:A:13:ALA:HB3	1:A:16:HIS:HD2	1.55	0.71
1:G:73:ALA:O	1:G:76:SER:HB3	1.90	0.71
1:E:13:ALA:HB3	1:E:16:HIS:CD2	2.24	0.71
1:D:13:ALA:HB3	1:D:16:HIS:O	1.90	0.71
1:E:66:GLU:O	1:E:70:LEU:HD13	1.91	0.71
1:H:155:VAL:HG12	1:H:156:GLU:N	2.03	0.71
1:E:77:VAL:HG12	1:E:78:SER:N	2.06	0.71
1:G:66:GLU:O	1:G:70:LEU:HD13	1.91	0.71
1:D:194:ALA:O	1:D:197:SER:HB3	1.91	0.71
1:D:156:GLU:O	1:D:160:GLY:N	2.22	0.71
1:F:13:ALA:HB3	1:F:16:HIS:O	1.89	0.71
1:G:70:LEU:O	1:G:73:ALA:HB3	1.89	0.71
1:C:77:VAL:HG12	1:C:78:SER:N	2.06	0.71
1:G:193:ARG:NH2	1:G:194:ALA:HB2	2.06	0.70
1:B:155:VAL:HG12	1:B:156:GLU:N	2.03	0.70
1:B:126:GLU:O	1:B:127:LEU:HG	1.92	0.70
1:B:187:ALA:O	1:B:189:SER:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:GLU:O	1:H:127:LEU:HG	1.92	0.70
1:D:187:ALA:O	1:D:189:SER:N	2.24	0.70
1:D:3:PHE:C	1:D:48:THR:HB	2.10	0.70
1:A:66:GLU:O	1:A:70:LEU:HD13	1.91	0.70
1:D:87:ALA:O	1:D:90:ALA:HB3	1.91	0.70
1:H:187:ALA:O	1:H:189:SER:N	2.24	0.70
1:B:101:LEU:HD21	1:B:127:LEU:HB3	1.74	0.69
1:B:104:SER:OG	1:B:104:SER:O	2.11	0.69
1:A:193:ARG:NH2	1:A:194:ALA:HB2	2.07	0.69
1:F:161:LEU:N	1:F:161:LEU:CD2	2.55	0.69
1:H:156:GLU:O	1:H:160:GLY:N	2.23	0.69
1:D:126:GLU:O	1:D:127:LEU:HG	1.93	0.69
1:C:29:ASN:HD21	1:C:60:TYR:HE1	1.41	0.69
1:F:104:SER:O	1:F:104:SER:OG	2.10	0.69
1:B:120:ALA:O	1:B:124:VAL:HG23	1.93	0.69
1:A:29:ASN:HD21	1:A:60:TYR:HE1	1.41	0.69
1:F:83:ARG:CB	1:F:84:LEU:HD12	2.21	0.69
1:E:110:THR:HA	1:E:115:ILE:HG22	1.75	0.69
1:B:87:ALA:O	1:B:90:ALA:HB3	1.92	0.69
1:G:110:THR:HA	1:G:115:ILE:HG22	1.75	0.69
1:F:101:LEU:HD21	1:F:127:LEU:HB3	1.75	0.69
1:D:104:SER:O	1:D:104:SER:OG	2.10	0.69
1:F:187:ALA:O	1:F:189:SER:N	2.25	0.69
1:C:99:GLN:O	1:C:101:LEU:O	2.11	0.69
1:F:173:ASP:O	1:F:175:VAL:N	2.26	0.69
1:E:130:LYS:HD2	1:E:134:VAL:HB	1.75	0.69
1:E:29:ASN:HD21	1:E:60:TYR:HE1	1.41	0.69
1:G:99:GLN:O	1:G:101:LEU:O	2.10	0.69
1:G:29:ASN:HD21	1:G:60:TYR:HE1	1.40	0.69
1:H:87:ALA:O	1:H:90:ALA:HB3	1.92	0.69
1:G:176:LEU:HG	1:G:177:ASP:CG	2.13	0.69
1:F:156:GLU:O	1:F:160:GLY:N	2.22	0.69
1:A:99:GLN:O	1:A:101:LEU:O	2.11	0.69
1:H:46:LEU:HD12	1:H:46:LEU:C	2.14	0.69
1:H:120:ALA:O	1:H:124:VAL:HG23	1.93	0.69
1:B:68:ARG:O	1:B:71:PHE:HB3	1.93	0.68
1:E:193:ARG:NH2	1:E:194:ALA:HB2	2.08	0.68
1:B:31:THR:HG22	1:B:86:MET:HE1	1.75	0.68
1:F:126:GLU:O	1:F:127:LEU:HG	1.93	0.68
1:E:77:VAL:O	1:E:80:VAL:HG12	1.93	0.68
1:B:48:THR:CG2	1:B:49:ALA:N	2.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:GLN:O	1:E:101:LEU:O	2.11	0.68
1:D:48:THR:CG2	1:D:49:ALA:N	2.56	0.68
1:F:87:ALA:O	1:F:90:ALA:HB3	1.92	0.68
1:B:91:VAL:CG1	1:B:92:HIS:H	1.89	0.68
1:C:176:LEU:HG	1:C:177:ASP:CG	2.12	0.68
1:B:173:ASP:O	1:B:175:VAL:N	2.27	0.68
1:H:161:LEU:N	1:H:161:LEU:CD2	2.56	0.68
1:D:120:ALA:O	1:D:124:VAL:HG23	1.94	0.68
1:H:173:ASP:O	1:H:175:VAL:N	2.27	0.68
1:D:31:THR:C	1:D:35:LEU:HD12	2.14	0.68
1:H:48:THR:CG2	1:H:49:ALA:N	2.56	0.68
1:G:77:VAL:O	1:G:80:VAL:HG12	1.94	0.68
1:C:77:VAL:O	1:C:80:VAL:HG12	1.93	0.68
1:G:130:LYS:HD2	1:G:134:VAL:HB	1.75	0.68
1:D:101:LEU:HD21	1:D:127:LEU:HB3	1.76	0.68
1:H:104:SER:O	1:H:104:SER:OG	2.09	0.68
1:E:154:VAL:HA	1:E:192:LEU:HD23	1.76	0.68
1:A:176:LEU:HG	1:A:177:ASP:CG	2.14	0.68
1:C:193:ARG:NH2	1:C:194:ALA:HB2	2.07	0.68
1:D:68:ARG:O	1:D:71:PHE:HB3	1.93	0.68
1:F:48:THR:CG2	1:F:49:ALA:N	2.57	0.68
1:H:83:ARG:CB	1:H:84:LEU:HD12	2.22	0.68
1:D:112:VAL:CG2	1:D:115:ILE:HB	2.24	0.68
1:H:101:LEU:HD21	1:H:127:LEU:HB3	1.75	0.68
1:A:193:ARG:CA	1:A:196:LEU:HG	2.24	0.68
1:F:31:THR:C	1:F:35:LEU:HD12	2.15	0.68
1:D:83:ARG:CB	1:D:84:LEU:HD12	2.21	0.68
1:F:35:LEU:HA	1:F:38:LEU:HD23	1.76	0.68
1:F:112:VAL:CG2	1:F:115:ILE:HB	2.24	0.68
1:B:112:VAL:CG2	1:B:115:ILE:HB	2.24	0.68
1:E:176:LEU:HG	1:E:177:ASP:CG	2.14	0.68
1:D:105:ASP:OD1	1:D:108:SER:N	2.27	0.67
1:C:193:ARG:CA	1:C:196:LEU:HG	2.24	0.67
1:C:196:LEU:HD12	1:C:197:SER:N	2.09	0.67
1:A:77:VAL:O	1:A:80:VAL:HG12	1.93	0.67
1:E:61:GLY:C	1:E:62:PHE:CD1	2.67	0.67
1:B:161:LEU:CD2	1:B:161:LEU:N	2.56	0.67
1:B:156:GLU:O	1:B:160:GLY:N	2.24	0.67
1:A:130:LYS:HD2	1:A:134:VAL:HB	1.74	0.67
1:C:130:LYS:HD2	1:C:134:VAL:HB	1.74	0.67
1:F:105:ASP:OD1	1:F:108:SER:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASP:OD1	1:B:108:SER:N	2.27	0.67
1:B:99:GLN:O	1:B:102:ALA:N	2.27	0.67
1:G:154:VAL:HA	1:G:192:LEU:HD23	1.77	0.67
1:C:176:LEU:HG	1:C:177:ASP:OD1	1.95	0.67
1:F:113:PRO:C	1:F:115:ILE:H	1.98	0.67
1:C:77:VAL:HG13	1:C:126:GLU:HG3	1.77	0.67
1:B:113:PRO:C	1:B:115:ILE:H	1.98	0.67
1:H:112:VAL:CG2	1:H:115:ILE:HB	2.24	0.67
1:H:113:PRO:C	1:H:115:ILE:H	1.98	0.67
1:A:176:LEU:HG	1:A:177:ASP:OD1	1.95	0.67
1:C:16:HIS:HA	1:C:29:ASN:HA	1.76	0.67
1:H:31:THR:C	1:H:35:LEU:HD12	2.15	0.67
1:E:77:VAL:HG13	1:E:126:GLU:HG3	1.76	0.67
1:C:110:THR:HA	1:C:115:ILE:HG22	1.75	0.67
1:D:46:LEU:C	1:D:46:LEU:HD12	2.15	0.67
1:F:46:LEU:C	1:F:46:LEU:HD12	2.15	0.67
1:F:39:ASN:O	1:F:42:SER:HB3	1.94	0.67
1:G:16:HIS:HA	1:G:29:ASN:HA	1.76	0.67
1:A:112:VAL:HG13	1:A:113:PRO:HD2	1.77	0.67
1:D:113:PRO:C	1:D:115:ILE:H	1.98	0.67
1:C:61:GLY:C	1:C:62:PHE:CD1	2.68	0.67
1:B:39:ASN:O	1:B:42:SER:HB3	1.95	0.67
1:D:66:GLU:OE1	1:D:66:GLU:N	2.27	0.67
1:B:46:LEU:C	1:B:46:LEU:HD12	2.15	0.67
1:D:35:LEU:HA	1:D:38:LEU:HD23	1.76	0.67
1:G:29:ASN:OD1	1:G:60:TYR:HD1	1.77	0.67
1:A:196:LEU:HD12	1:A:197:SER:N	2.09	0.67
1:G:176:LEU:HG	1:G:177:ASP:OD1	1.95	0.67
1:D:39:ASN:O	1:D:42:SER:HB3	1.95	0.67
1:D:173:ASP:O	1:D:175:VAL:N	2.28	0.66
1:B:78:SER:O	1:B:80:VAL:HG22	1.96	0.66
1:F:68:ARG:O	1:F:71:PHE:HB3	1.94	0.66
1:F:95:ALA:O	1:F:96:ALA:C	2.33	0.66
1:H:105:ASP:OD1	1:H:108:SER:N	2.28	0.66
1:G:4:SER:O	1:G:5:VAL:CG2	2.40	0.66
1:D:78:SER:O	1:D:80:VAL:HG22	1.95	0.66
1:H:68:ARG:O	1:H:71:PHE:HB3	1.94	0.66
1:G:80:VAL:O	1:G:80:VAL:HG13	1.95	0.66
1:F:66:GLU:N	1:F:66:GLU:OE1	2.28	0.66
1:H:35:LEU:HA	1:H:38:LEU:HD23	1.78	0.66
1:A:61:GLY:C	1:A:62:PHE:CD1	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:LEU:HD12	1:E:197:SER:N	2.10	0.66
1:C:112:VAL:HG13	1:C:113:PRO:HD2	1.77	0.66
1:A:110:THR:HA	1:A:115:ILE:HG22	1.76	0.66
1:E:176:LEU:HG	1:E:177:ASP:OD1	1.95	0.66
1:D:161:LEU:CD2	1:D:161:LEU:N	2.56	0.66
1:D:199:LEU:H	1:D:199:LEU:HD12	1.60	0.66
1:E:29:ASN:OD1	1:E:60:TYR:HD1	1.78	0.66
1:F:78:SER:O	1:F:80:VAL:HG22	1.96	0.66
1:H:91:VAL:CG1	1:H:92:HIS:H	1.89	0.66
1:B:31:THR:C	1:B:35:LEU:HD12	2.16	0.66
1:B:68:ARG:HG3	1:B:69:ASP:N	2.11	0.66
1:A:77:VAL:HG13	1:A:126:GLU:HG3	1.78	0.66
1:G:77:VAL:HG13	1:G:126:GLU:HG3	1.77	0.66
1:G:61:GLY:C	1:G:62:PHE:CD1	2.69	0.66
1:B:83:ARG:CB	1:B:84:LEU:HD12	2.21	0.66
1:B:31:THR:HG22	1:B:86:MET:HE3	1.78	0.66
1:F:120:ALA:O	1:F:124:VAL:HG23	1.95	0.66
1:E:80:VAL:HG13	1:E:80:VAL:O	1.95	0.66
1:C:80:VAL:HG13	1:C:80:VAL:O	1.95	0.66
1:G:196:LEU:HD12	1:G:197:SER:N	2.09	0.66
1:F:199:LEU:H	1:F:199:LEU:HD12	1.60	0.66
1:G:70:LEU:HA	1:G:73:ALA:HB3	1.78	0.66
1:D:99:GLN:O	1:D:102:ALA:N	2.29	0.66
1:B:95:ALA:O	1:B:96:ALA:C	2.33	0.66
1:A:29:ASN:OD1	1:A:60:TYR:HD1	1.78	0.65
1:F:99:GLN:O	1:F:102:ALA:N	2.30	0.65
1:E:16:HIS:HA	1:E:29:ASN:HA	1.78	0.65
1:H:95:ALA:O	1:H:96:ALA:C	2.34	0.65
1:G:193:ARG:CA	1:G:196:LEU:HG	2.25	0.65
1:H:39:ASN:O	1:H:42:SER:HB3	1.96	0.65
1:H:84:LEU:O	1:H:85:ALA:C	2.34	0.65
1:A:70:LEU:HA	1:A:73:ALA:HB3	1.78	0.65
1:H:99:GLN:O	1:H:102:ALA:N	2.29	0.65
1:G:166:LYS:H	1:G:166:LYS:HD2	1.60	0.65
1:C:29:ASN:OD1	1:C:60:TYR:HD1	1.78	0.65
1:A:154:VAL:HA	1:A:192:LEU:HD23	1.77	0.65
1:A:166:LYS:H	1:A:166:LYS:HD2	1.61	0.65
1:C:18:VAL:HA	1:C:26:TYR:O	1.95	0.65
1:A:16:HIS:HA	1:A:29:ASN:HA	1.77	0.65
1:C:154:VAL:HA	1:C:192:LEU:HD23	1.77	0.65
1:E:166:LYS:HD2	1:E:166:LYS:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:VAL:CG1	1:D:78:SER:N	2.60	0.65
1:B:3:PHE:O	1:B:48:THR:HB	1.97	0.65
1:E:18:VAL:HA	1:E:26:TYR:O	1.97	0.65
1:F:84:LEU:O	1:F:85:ALA:C	2.35	0.65
1:A:80:VAL:HG13	1:A:80:VAL:O	1.95	0.65
1:C:70:LEU:HA	1:C:73:ALA:HB3	1.79	0.65
1:H:199:LEU:H	1:H:199:LEU:HD12	1.61	0.65
1:E:112:VAL:HG13	1:E:113:PRO:HD2	1.77	0.65
1:D:95:ALA:O	1:D:96:ALA:C	2.34	0.65
1:F:3:PHE:O	1:F:48:THR:HB	1.97	0.65
1:G:18:VAL:HA	1:G:26:TYR:O	1.96	0.65
1:C:153:SER:C	1:C:155:VAL:N	2.51	0.65
1:E:70:LEU:HA	1:E:73:ALA:HB3	1.78	0.65
1:B:35:LEU:HA	1:B:38:LEU:HD23	1.78	0.64
1:C:4:SER:O	1:C:5:VAL:CG2	2.41	0.64
1:B:199:LEU:HD12	1:B:199:LEU:H	1.61	0.64
1:C:171:ALA:O	1:C:174:GLN:HB3	1.97	0.64
1:H:77:VAL:CG1	1:H:78:SER:N	2.60	0.64
1:H:66:GLU:N	1:H:66:GLU:OE1	2.28	0.64
1:D:77:VAL:CG1	1:D:78:SER:H	2.09	0.64
1:F:77:VAL:CG1	1:F:78:SER:N	2.60	0.64
1:H:78:SER:O	1:H:80:VAL:HG22	1.98	0.64
1:G:112:VAL:HG13	1:G:113:PRO:HD2	1.79	0.64
1:B:109:LEU:C	1:B:111:ARG:H	2.01	0.64
1:C:24:ILE:HG22	1:C:26:TYR:CE1	2.33	0.64
1:D:109:LEU:C	1:D:111:ARG:H	2.01	0.64
1:A:153:SER:C	1:A:155:VAL:N	2.51	0.64
1:C:166:LYS:HD2	1:C:166:LYS:H	1.61	0.64
1:E:171:ALA:O	1:E:174:GLN:HB3	1.97	0.64
1:B:66:GLU:OE1	1:B:66:GLU:N	2.27	0.64
1:E:24:ILE:HG22	1:E:26:TYR:CE1	2.33	0.64
1:F:77:VAL:CG1	1:F:78:SER:H	2.10	0.64
1:E:193:ARG:CA	1:E:196:LEU:HG	2.24	0.64
1:F:84:LEU:O	1:F:87:ALA:N	2.31	0.64
1:G:29:ASN:OD1	1:G:60:TYR:CD1	2.50	0.64
1:A:109:LEU:O	1:A:111:ARG:N	2.31	0.64
1:E:193:ARG:HA	1:E:196:LEU:CD2	2.28	0.64
1:D:64:ASP:OD1	1:D:67:ASN:N	2.28	0.64
1:A:29:ASN:OD1	1:A:60:TYR:CD1	2.51	0.64
1:B:84:LEU:O	1:B:85:ALA:C	2.36	0.64
1:F:125:LEU:HD23	1:F:126:GLU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:LEU:HD23	1:H:126:GLU:N	2.13	0.64
1:C:28:VAL:O	1:C:28:VAL:HG13	1.98	0.64
1:C:29:ASN:OD1	1:C:60:TYR:CD1	2.51	0.63
1:F:109:LEU:C	1:F:111:ARG:H	2.00	0.63
1:F:64:ASP:OD1	1:F:67:ASN:N	2.28	0.63
1:H:112:VAL:HG22	1:H:115:ILE:HB	1.81	0.63
1:F:64:ASP:HB2	1:F:66:GLU:OE1	1.99	0.63
1:D:3:PHE:O	1:D:48:THR:HB	1.99	0.63
1:H:3:PHE:O	1:H:48:THR:HB	1.98	0.63
1:F:91:VAL:CG1	1:F:92:HIS:H	1.89	0.63
1:D:125:LEU:HD23	1:D:126:GLU:N	2.13	0.63
1:H:77:VAL:CG1	1:H:78:SER:H	2.10	0.63
1:C:91:VAL:CG1	1:C:92:HIS:CD2	2.76	0.63
1:B:14:LEU:CD1	1:B:14:LEU:H	2.10	0.63
1:A:158:LEU:CD2	1:A:158:LEU:H	2.11	0.63
1:G:171:ALA:O	1:G:174:GLN:HB3	1.98	0.63
1:G:109:LEU:O	1:G:111:ARG:N	2.31	0.63
1:H:109:LEU:C	1:H:111:ARG:H	2.01	0.63
1:E:28:VAL:O	1:E:28:VAL:HG13	1.96	0.63
1:D:84:LEU:O	1:D:85:ALA:C	2.36	0.63
1:B:77:VAL:CG1	1:B:78:SER:H	2.11	0.63
1:E:109:LEU:O	1:E:111:ARG:N	2.31	0.63
1:A:193:ARG:HA	1:A:196:LEU:CD2	2.28	0.63
1:C:158:LEU:CD2	1:C:158:LEU:H	2.10	0.63
1:C:193:ARG:HA	1:C:196:LEU:CD2	2.27	0.63
1:C:109:LEU:O	1:C:111:ARG:N	2.32	0.63
1:E:46:LEU:O	1:E:47:VAL:C	2.36	0.63
1:A:24:ILE:HG22	1:A:26:TYR:CE1	2.33	0.63
1:E:29:ASN:OD1	1:E:60:TYR:CD1	2.51	0.63
1:F:94:ALA:O	1:F:96:ALA:N	2.32	0.63
1:A:171:ALA:O	1:A:174:GLN:HB3	1.99	0.63
1:D:84:LEU:O	1:D:87:ALA:N	2.32	0.63
1:F:68:ARG:HG3	1:F:69:ASP:N	2.12	0.63
1:G:101:LEU:O	1:G:102:ALA:HB3	1.99	0.63
1:A:101:LEU:O	1:A:102:ALA:HB3	1.99	0.63
1:A:18:VAL:HA	1:A:26:TYR:O	1.98	0.62
1:B:64:ASP:OD1	1:B:67:ASN:N	2.28	0.62
1:G:28:VAL:HG13	1:G:28:VAL:O	1.98	0.62
1:A:202:THR:O	1:D:108:SER:HB2	1.99	0.62
1:D:112:VAL:HG22	1:D:115:ILE:HB	1.80	0.62
1:H:94:ALA:O	1:H:96:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ARG:HA	1:G:196:LEU:CD2	2.28	0.62
1:A:28:VAL:HG13	1:A:28:VAL:O	1.99	0.62
1:D:94:ALA:O	1:D:96:ALA:N	2.33	0.62
1:H:130:LYS:O	1:H:131:VAL:CB	2.47	0.62
1:A:46:LEU:O	1:A:47:VAL:C	2.37	0.62
1:E:4:SER:O	1:E:5:VAL:CG2	2.41	0.62
1:E:101:LEU:O	1:E:102:ALA:HB3	1.99	0.62
1:F:112:VAL:HG22	1:F:115:ILE:HB	1.81	0.62
1:B:94:ALA:O	1:B:96:ALA:N	2.33	0.62
1:F:19:ILE:O	1:F:25:GLY:HA2	2.00	0.62
1:H:68:ARG:HG3	1:H:69:ASP:N	2.12	0.62
1:H:84:LEU:O	1:H:87:ALA:N	2.33	0.62
1:G:153:SER:C	1:G:155:VAL:N	2.51	0.62
1:F:97:LEU:O	1:F:98:ARG:C	2.37	0.62
1:B:112:VAL:HG22	1:B:115:ILE:HB	1.81	0.62
1:E:158:LEU:H	1:E:158:LEU:CD2	2.11	0.62
1:B:64:ASP:HB2	1:B:66:GLU:OE1	2.00	0.62
1:A:173:ASP:CG	1:A:176:LEU:HD23	2.20	0.62
1:G:158:LEU:CD2	1:G:158:LEU:H	2.12	0.62
1:C:173:ASP:CG	1:C:176:LEU:HD23	2.20	0.62
1:D:64:ASP:HB2	1:D:66:GLU:OE1	1.98	0.62
1:B:19:ILE:O	1:B:25:GLY:HA2	2.00	0.62
1:F:189:SER:C	1:F:191:ALA:N	2.52	0.62
1:C:101:LEU:O	1:C:102:ALA:HB3	1.99	0.62
1:B:97:LEU:O	1:B:98:ARG:C	2.38	0.62
1:H:64:ASP:HB2	1:H:66:GLU:OE1	2.00	0.62
1:C:158:LEU:HD22	1:C:158:LEU:N	2.15	0.61
1:E:173:ASP:CG	1:E:176:LEU:HD23	2.21	0.61
1:G:24:ILE:HG22	1:G:26:TYR:CE1	2.35	0.61
1:E:70:LEU:HA	1:E:73:ALA:CB	2.30	0.61
1:F:130:LYS:O	1:F:131:VAL:CB	2.47	0.61
1:E:74:LEU:O	1:E:80:VAL:HG11	2.01	0.61
1:D:14:LEU:H	1:D:14:LEU:CD1	2.10	0.61
1:E:158:LEU:N	1:E:158:LEU:HD22	2.16	0.61
1:F:154:VAL:O	1:F:157:ALA:HB3	2.00	0.61
1:A:74:LEU:O	1:A:80:VAL:HG11	2.00	0.61
1:B:125:LEU:HD23	1:B:126:GLU:N	2.15	0.61
1:F:173:ASP:O	1:F:174:GLN:C	2.39	0.61
1:E:77:VAL:HB	1:E:80:VAL:CG1	2.31	0.61
1:A:77:VAL:HB	1:A:80:VAL:CG1	2.31	0.61
1:A:4:SER:O	1:A:5:VAL:CG2	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:154:VAL:O	1:H:157:ALA:HB3	2.00	0.61
1:G:70:LEU:HA	1:G:73:ALA:CB	2.31	0.61
1:E:91:VAL:CG1	1:E:92:HIS:CD2	2.76	0.61
1:A:158:LEU:N	1:A:158:LEU:HD22	2.15	0.61
1:E:153:SER:C	1:E:155:VAL:N	2.51	0.61
1:B:108:SER:HB2	1:C:202:THR:O	2.01	0.61
1:H:19:ILE:O	1:H:25:GLY:HA2	2.01	0.61
1:B:84:LEU:O	1:B:87:ALA:N	2.34	0.61
1:E:18:VAL:O	1:E:18:VAL:HG23	2.01	0.61
1:C:77:VAL:HB	1:C:80:VAL:CG1	2.31	0.61
1:B:154:VAL:O	1:B:157:ALA:HB3	2.00	0.61
1:D:19:ILE:O	1:D:25:GLY:HA2	2.01	0.60
1:A:70:LEU:HA	1:A:73:ALA:CB	2.30	0.60
1:D:15:ASP:N	1:D:15:ASP:OD1	2.24	0.60
1:A:91:VAL:CG1	1:A:92:HIS:CD2	2.76	0.60
1:G:77:VAL:HB	1:G:80:VAL:CG1	2.31	0.60
1:D:97:LEU:O	1:D:98:ARG:C	2.38	0.60
1:C:46:LEU:O	1:C:47:VAL:C	2.37	0.60
1:G:173:ASP:CG	1:G:176:LEU:HD23	2.21	0.60
1:G:158:LEU:HD22	1:G:158:LEU:N	2.16	0.60
1:B:15:ASP:N	1:B:15:ASP:OD1	2.23	0.60
1:H:97:LEU:O	1:H:98:ARG:C	2.38	0.60
1:G:188:THR:O	1:G:191:ALA:HB3	2.01	0.60
1:D:154:VAL:O	1:D:157:ALA:HB3	2.00	0.60
1:D:68:ARG:HG3	1:D:69:ASP:N	2.11	0.60
1:B:24:ILE:HG22	1:B:25:GLY:N	2.16	0.60
1:G:91:VAL:CG1	1:G:92:HIS:CD2	2.76	0.60
1:E:61:GLY:O	1:E:62:PHE:CD1	2.55	0.60
1:C:70:LEU:HA	1:C:73:ALA:CB	2.31	0.60
1:C:74:LEU:O	1:C:80:VAL:HG11	2.02	0.60
1:D:24:ILE:HG22	1:D:25:GLY:N	2.16	0.60
1:F:129:ASP:CG	1:F:130:LYS:N	2.55	0.60
1:C:18:VAL:O	1:C:18:VAL:HG23	2.01	0.60
1:G:126:GLU:CA	1:G:126:GLU:OE1	2.50	0.60
1:E:113:PRO:O	1:E:114:GLY:C	2.40	0.60
1:H:189:SER:C	1:H:191:ALA:N	2.54	0.60
1:A:188:THR:O	1:A:191:ALA:HB3	2.02	0.60
1:B:77:VAL:CG1	1:B:78:SER:N	2.61	0.60
1:G:193:ARG:CZ	1:G:194:ALA:HB2	2.32	0.59
1:B:173:ASP:O	1:B:174:GLN:C	2.39	0.59
1:G:74:LEU:O	1:G:80:VAL:HG11	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:ASP:O	1:G:97:LEU:HB2	2.01	0.59
1:A:93:ASP:O	1:A:97:LEU:HB2	2.02	0.59
1:H:173:ASP:O	1:H:174:GLN:C	2.40	0.59
1:A:31:THR:O	1:A:34:ALA:N	2.35	0.59
1:H:119:GLY:O	1:H:123:ILE:HG12	2.02	0.59
1:B:104:SER:O	1:B:106:VAL:HG23	2.03	0.59
1:H:99:GLN:O	1:H:101:LEU:N	2.36	0.59
1:E:188:THR:O	1:E:191:ALA:HB3	2.02	0.59
1:C:113:PRO:O	1:C:114:GLY:C	2.39	0.59
1:C:93:ASP:C	1:C:93:ASP:OD1	2.41	0.59
1:F:108:SER:HB2	1:G:202:THR:O	2.02	0.59
1:D:125:LEU:O	1:D:125:LEU:HG	2.03	0.59
1:C:127:LEU:O	1:C:129:ASP:N	2.36	0.59
1:G:18:VAL:O	1:G:18:VAL:HG23	2.01	0.59
1:F:110:THR:HA	1:F:115:ILE:CG2	2.33	0.59
1:F:119:GLY:O	1:F:123:ILE:HG12	2.02	0.59
1:B:119:GLY:O	1:B:123:ILE:HG12	2.03	0.59
1:H:64:ASP:OD1	1:H:67:ASN:N	2.29	0.59
1:E:126:GLU:OE1	1:E:126:GLU:CA	2.50	0.59
1:B:129:ASP:CG	1:B:130:LYS:N	2.55	0.59
1:G:102:ALA:C	1:G:104:SER:H	2.06	0.59
1:D:6:ARG:HB2	1:D:45:ARG:HB2	1.85	0.59
1:E:19:ILE:HD13	1:E:19:ILE:N	2.18	0.59
1:D:129:ASP:CG	1:D:130:LYS:N	2.55	0.59
1:E:93:ASP:O	1:E:97:LEU:HB2	2.02	0.59
1:H:129:ASP:CG	1:H:130:LYS:N	2.55	0.58
1:G:127:LEU:O	1:G:129:ASP:N	2.36	0.58
1:D:173:ASP:O	1:D:174:GLN:C	2.40	0.58
1:A:18:VAL:HG23	1:A:18:VAL:O	2.03	0.58
1:G:113:PRO:O	1:G:114:GLY:C	2.40	0.58
1:C:93:ASP:O	1:C:97:LEU:HB2	2.03	0.58
1:A:93:ASP:C	1:A:93:ASP:OD1	2.42	0.58
1:F:151:ARG:NH1	1:F:173:ASP:OD1	2.35	0.58
1:H:110:THR:HA	1:H:115:ILE:CG2	2.34	0.58
1:H:5:VAL:HG12	1:H:5:VAL:O	2.03	0.58
1:C:19:ILE:N	1:C:19:ILE:HD13	2.18	0.58
1:F:48:THR:O	1:F:68:ARG:HD3	2.04	0.58
1:G:46:LEU:O	1:G:47:VAL:C	2.37	0.58
1:E:193:ARG:CZ	1:E:194:ALA:HB2	2.34	0.58
1:C:188:THR:O	1:C:191:ALA:HB3	2.04	0.58
1:G:176:LEU:HG	1:G:177:ASP:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:ASP:C	1:G:93:ASP:OD1	2.41	0.58
1:H:6:ARG:HB2	1:H:45:ARG:HB2	1.85	0.58
1:B:6:ARG:HB2	1:B:45:ARG:HB2	1.86	0.58
1:D:119:GLY:O	1:D:123:ILE:HG12	2.02	0.58
1:D:5:VAL:O	1:D:5:VAL:HG12	2.03	0.58
1:F:24:ILE:HG22	1:F:25:GLY:N	2.18	0.58
1:A:176:LEU:HG	1:A:177:ASP:N	2.17	0.58
1:C:176:LEU:HG	1:C:177:ASP:N	2.17	0.58
1:D:73:ALA:O	1:D:74:LEU:C	2.42	0.58
1:C:61:GLY:O	1:C:62:PHE:CD1	2.55	0.58
1:E:176:LEU:HG	1:E:177:ASP:N	2.17	0.58
1:E:102:ALA:C	1:E:104:SER:H	2.06	0.58
1:D:70:LEU:N	1:D:70:LEU:CD2	2.66	0.58
1:H:15:ASP:OD1	1:H:15:ASP:N	2.23	0.58
1:H:24:ILE:HG22	1:H:25:GLY:N	2.17	0.58
1:D:70:LEU:C	1:D:74:LEU:HD12	2.24	0.58
1:D:72:LEU:O	1:D:75:LEU:HB3	2.03	0.58
1:H:84:LEU:O	1:H:86:MET:N	2.36	0.58
1:A:65:ALA:O	1:A:66:GLU:C	2.41	0.58
1:G:61:GLY:O	1:G:62:PHE:CD1	2.57	0.58
1:A:193:ARG:CZ	1:A:194:ALA:HB2	2.33	0.58
1:E:93:ASP:C	1:E:93:ASP:OD1	2.41	0.58
1:D:84:LEU:O	1:D:86:MET:N	2.37	0.58
1:E:202:THR:O	1:H:108:SER:HB2	2.04	0.58
1:H:151:ARG:NH1	1:H:173:ASP:OD1	2.36	0.58
1:E:31:THR:O	1:E:34:ALA:N	2.36	0.58
1:C:148:ASN:HA	1:C:151:ARG:HD2	1.86	0.58
1:B:70:LEU:CD2	1:B:70:LEU:N	2.65	0.58
1:B:72:LEU:O	1:B:75:LEU:HB3	2.04	0.58
1:H:31:THR:HG22	1:H:86:MET:HE3	1.85	0.58
1:G:65:ALA:O	1:G:66:GLU:C	2.41	0.58
1:C:65:ALA:O	1:C:66:GLU:C	2.42	0.58
1:B:110:THR:HA	1:B:115:ILE:CG2	2.33	0.58
1:G:3:PHE:O	1:G:48:THR:N	2.36	0.58
1:B:151:ARG:NH1	1:B:173:ASP:OD1	2.37	0.58
1:D:151:ARG:NH1	1:D:173:ASP:OD1	2.37	0.58
1:F:99:GLN:O	1:F:101:LEU:N	2.37	0.57
1:F:104:SER:O	1:F:106:VAL:HG23	2.03	0.57
1:D:189:SER:C	1:D:191:ALA:N	2.53	0.57
1:H:201:LYS:HE2	1:H:202:THR:OG1	2.04	0.57
1:H:167:GLN:NE2	1:H:167:GLN:CA	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:D:57:MET:O	2.03	0.57
1:A:19:ILE:N	1:A:19:ILE:HD13	2.18	0.57
1:F:84:LEU:O	1:F:86:MET:N	2.36	0.57
1:G:77:VAL:HG12	1:G:78:SER:O	2.04	0.57
1:H:95:ALA:O	1:H:98:ARG:N	2.37	0.57
1:A:3:PHE:O	1:A:48:THR:N	2.35	0.57
1:D:95:ALA:O	1:D:98:ARG:N	2.37	0.57
1:A:127:LEU:O	1:A:129:ASP:N	2.35	0.57
1:H:14:LEU:N	1:H:14:LEU:HD12	2.12	0.57
1:F:70:LEU:C	1:F:74:LEU:HD12	2.24	0.57
1:B:99:GLN:O	1:B:101:LEU:N	2.36	0.57
1:B:167:GLN:CA	1:B:167:GLN:NE2	2.67	0.57
1:D:48:THR:O	1:D:68:ARG:HD3	2.04	0.57
1:B:70:LEU:C	1:B:74:LEU:HD12	2.24	0.57
1:E:24:ILE:HD11	1:F:26:TYR:CE1	2.40	0.57
1:H:72:LEU:O	1:H:75:LEU:HB3	2.04	0.57
1:A:113:PRO:O	1:A:114:GLY:C	2.40	0.57
1:D:104:SER:O	1:D:106:VAL:HG23	2.04	0.57
1:C:155:VAL:CA	1:C:158:LEU:HD23	2.35	0.57
1:H:165:ALA:O	1:H:166:LYS:C	2.43	0.57
1:G:148:ASN:HA	1:G:151:ARG:HD2	1.86	0.57
1:A:114:GLY:O	1:A:115:ILE:HG12	2.04	0.57
1:E:85:ALA:O	1:E:86:MET:C	2.43	0.57
1:E:148:ASN:HA	1:E:151:ARG:HD2	1.86	0.57
1:D:113:PRO:O	1:D:115:ILE:N	2.38	0.57
1:C:110:THR:O	1:C:112:VAL:N	2.38	0.57
1:F:165:ALA:O	1:F:166:LYS:C	2.43	0.57
1:C:102:ALA:C	1:C:104:SER:H	2.06	0.57
1:A:61:GLY:O	1:A:62:PHE:CD1	2.57	0.57
1:C:3:PHE:O	1:C:48:THR:N	2.37	0.57
1:C:61:GLY:O	1:C:62:PHE:CG	2.57	0.57
1:C:31:THR:O	1:C:34:ALA:N	2.35	0.57
1:G:31:THR:C	1:G:35:LEU:HD12	2.25	0.57
1:B:48:THR:O	1:B:68:ARG:HD3	2.05	0.57
1:F:72:LEU:O	1:F:75:LEU:HB3	2.04	0.57
1:H:70:LEU:C	1:H:74:LEU:HD12	2.25	0.57
1:H:109:LEU:C	1:H:111:ARG:N	2.58	0.57
1:C:193:ARG:CZ	1:C:194:ALA:HB2	2.34	0.57
1:G:24:ILE:HD11	1:H:26:TYR:CE1	2.40	0.57
1:G:115:ILE:O	1:G:115:ILE:CG2	2.52	0.57
1:H:113:PRO:O	1:H:115:ILE:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ASN:HD22	1:D:29:ASN:H	1.53	0.57
1:B:157:ALA:O	1:B:160:GLY:N	2.38	0.57
1:F:70:LEU:CD2	1:F:70:LEU:N	2.64	0.56
1:H:48:THR:O	1:H:68:ARG:HD3	2.04	0.56
1:A:112:VAL:CG1	1:A:113:PRO:HD2	2.35	0.56
1:A:115:ILE:CG2	1:A:115:ILE:O	2.53	0.56
1:G:114:GLY:O	1:G:115:ILE:HG12	2.05	0.56
1:B:113:PRO:O	1:B:115:ILE:N	2.38	0.56
1:H:104:SER:O	1:H:106:VAL:HG23	2.05	0.56
1:G:176:LEU:CG	1:G:177:ASP:N	2.68	0.56
1:B:201:LYS:HE2	1:B:202:THR:OG1	2.05	0.56
1:F:157:ALA:O	1:F:160:GLY:N	2.38	0.56
1:B:21:ALA:O	1:B:22:ALA:C	2.44	0.56
1:A:77:VAL:HG12	1:A:78:SER:O	2.04	0.56
1:E:127:LEU:O	1:E:129:ASP:N	2.35	0.56
1:B:166:LYS:HA	1:B:169:GLU:OE2	2.06	0.56
1:F:57:MET:O	1:G:1:MET:HB2	2.04	0.56
1:A:102:ALA:C	1:A:104:SER:H	2.06	0.56
1:D:82:PRO:O	1:D:86:MET:HB2	2.05	0.56
1:B:84:LEU:O	1:B:86:MET:N	2.38	0.56
1:A:110:THR:O	1:A:112:VAL:N	2.38	0.56
1:F:95:ALA:O	1:F:98:ARG:N	2.37	0.56
1:C:65:ALA:O	1:C:68:ARG:N	2.39	0.56
1:E:77:VAL:HG12	1:E:78:SER:O	2.05	0.56
1:E:110:THR:O	1:E:112:VAL:N	2.39	0.56
1:E:114:GLY:O	1:E:115:ILE:HG12	2.04	0.56
1:B:95:ALA:O	1:B:98:ARG:N	2.37	0.56
1:E:61:GLY:O	1:E:62:PHE:CG	2.58	0.56
1:G:129:ASP:O	1:G:131:VAL:N	2.34	0.56
1:B:189:SER:C	1:B:191:ALA:N	2.54	0.56
1:A:176:LEU:CG	1:A:177:ASP:N	2.68	0.56
1:C:104:SER:O	1:C:106:VAL:HG12	2.04	0.56
1:B:57:MET:O	1:C:1:MET:HB2	2.04	0.56
1:G:15:ASP:O	1:G:16:HIS:HB3	2.06	0.56
1:E:109:LEU:O	1:E:110:THR:C	2.44	0.56
1:F:201:LYS:HE2	1:F:202:THR:OG1	2.05	0.56
1:D:201:LYS:HE2	1:D:202:THR:OG1	2.05	0.56
1:G:54:GLU:CD	1:G:55:ASP:N	2.59	0.56
1:F:6:ARG:HB2	1:F:45:ARG:HB2	1.87	0.56
1:E:72:LEU:O	1:E:73:ALA:C	2.44	0.56
1:A:101:LEU:O	1:A:102:ALA:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:GLN:O	1:D:101:LEU:N	2.39	0.56
1:H:112:VAL:HG23	1:H:113:PRO:O	2.06	0.56
1:E:129:ASP:O	1:E:131:VAL:N	2.34	0.56
1:G:154:VAL:O	1:G:158:LEU:HD21	2.06	0.56
1:E:176:LEU:CG	1:E:177:ASP:N	2.68	0.56
1:D:167:GLN:CA	1:D:167:GLN:NE2	2.67	0.56
1:F:166:LYS:HA	1:F:169:GLU:OE2	2.06	0.56
1:E:1:MET:HB2	1:H:57:MET:O	2.06	0.56
1:F:5:VAL:O	1:F:5:VAL:HG12	2.06	0.56
1:D:31:THR:HG22	1:D:86:MET:HE3	1.85	0.56
1:G:110:THR:O	1:G:112:VAL:N	2.38	0.56
1:D:112:VAL:HG23	1:D:113:PRO:O	2.06	0.56
1:C:154:VAL:O	1:C:158:LEU:HD21	2.05	0.56
1:E:65:ALA:O	1:E:66:GLU:C	2.42	0.56
1:A:31:THR:C	1:A:35:LEU:HD12	2.26	0.56
1:E:31:THR:C	1:E:35:LEU:HD12	2.26	0.56
1:G:19:ILE:N	1:G:19:ILE:HD13	2.20	0.56
1:A:24:ILE:HD11	1:B:26:TYR:CE1	2.39	0.56
1:H:73:ALA:O	1:H:74:LEU:C	2.43	0.56
1:A:48:THR:HG22	1:A:61:GLY:HA2	1.88	0.56
1:H:29:ASN:H	1:H:29:ASN:HD22	1.54	0.56
1:C:114:GLY:O	1:C:115:ILE:HG12	2.06	0.56
1:H:21:ALA:O	1:H:22:ALA:C	2.44	0.56
1:H:82:PRO:O	1:H:86:MET:HB2	2.06	0.56
1:A:67:ASN:O	1:A:68:ARG:C	2.44	0.56
1:C:48:THR:HG22	1:C:61:GLY:HA2	1.88	0.56
1:H:191:ALA:O	1:H:192:LEU:C	2.44	0.56
1:C:176:LEU:CG	1:C:177:ASP:N	2.68	0.56
1:D:166:LYS:HA	1:D:169:GLU:OE2	2.06	0.56
1:B:165:ALA:O	1:B:166:LYS:C	2.43	0.56
1:A:54:GLU:CD	1:A:55:ASP:N	2.59	0.56
1:G:31:THR:O	1:G:34:ALA:N	2.36	0.56
1:A:148:ASN:HA	1:A:151:ARG:HD2	1.88	0.56
1:A:72:LEU:O	1:A:73:ALA:C	2.44	0.56
1:F:113:PRO:O	1:F:115:ILE:N	2.38	0.56
1:F:125:LEU:O	1:F:125:LEU:HG	2.06	0.56
1:C:71:PHE:HA	1:C:74:LEU:HD12	1.88	0.56
1:D:110:THR:HA	1:D:115:ILE:CG2	2.34	0.56
1:B:167:GLN:NE2	1:B:167:GLN:HA	2.21	0.56
1:A:104:SER:O	1:A:106:VAL:N	2.35	0.56
1:F:109:LEU:C	1:F:111:ARG:N	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:HG3	1:B:193:ARG:NH1	2.21	0.56
1:E:104:SER:O	1:E:106:VAL:HG12	2.06	0.56
1:A:106:VAL:O	1:A:107:ALA:C	2.44	0.56
1:G:85:ALA:O	1:G:86:MET:C	2.44	0.55
1:C:72:LEU:O	1:C:73:ALA:C	2.44	0.55
1:D:113:PRO:C	1:D:115:ILE:N	2.59	0.55
1:A:61:GLY:O	1:A:62:PHE:CG	2.59	0.55
1:D:193:ARG:NH1	1:D:193:ARG:HG3	2.21	0.55
1:C:112:VAL:CG1	1:C:113:PRO:HD2	2.36	0.55
1:E:15:ASP:O	1:E:16:HIS:HB3	2.06	0.55
1:G:109:LEU:O	1:G:110:THR:C	2.44	0.55
1:G:71:PHE:HA	1:G:74:LEU:HD12	1.88	0.55
1:E:71:PHE:HA	1:E:74:LEU:HD12	1.89	0.55
1:G:48:THR:HG22	1:G:61:GLY:HA2	1.89	0.55
1:C:101:LEU:O	1:C:102:ALA:CB	2.54	0.55
1:C:106:VAL:O	1:C:107:ALA:C	2.44	0.55
1:F:82:PRO:O	1:F:86:MET:HB2	2.05	0.55
1:A:65:ALA:O	1:A:68:ARG:N	2.39	0.55
1:A:85:ALA:O	1:A:86:MET:C	2.44	0.55
1:E:101:LEU:O	1:E:102:ALA:CB	2.54	0.55
1:D:21:ALA:O	1:D:22:ALA:C	2.44	0.55
1:F:16:HIS:CD2	1:F:27:ARG:HD3	2.41	0.55
1:D:109:LEU:C	1:D:111:ARG:N	2.58	0.55
1:B:125:LEU:HG	1:B:125:LEU:O	2.05	0.55
1:H:113:PRO:C	1:H:115:ILE:N	2.59	0.55
1:D:16:HIS:CD2	1:D:27:ARG:HD3	2.42	0.55
1:E:154:VAL:O	1:E:158:LEU:HD21	2.05	0.55
1:C:109:LEU:O	1:C:110:THR:C	2.45	0.55
1:G:65:ALA:O	1:G:68:ARG:N	2.39	0.55
1:E:112:VAL:CG1	1:E:113:PRO:HD2	2.36	0.55
1:A:129:ASP:O	1:A:131:VAL:N	2.34	0.55
1:D:157:ALA:O	1:D:160:GLY:N	2.39	0.55
1:F:167:GLN:HA	1:F:167:GLN:NE2	2.21	0.55
1:H:167:GLN:NE2	1:H:167:GLN:HA	2.21	0.55
1:A:104:SER:O	1:A:106:VAL:HG12	2.06	0.55
1:C:24:ILE:HD11	1:D:26:TYR:CE1	2.42	0.55
1:F:73:ALA:O	1:F:74:LEU:C	2.42	0.55
1:D:112:VAL:HG23	1:D:113:PRO:N	2.22	0.55
1:B:113:PRO:C	1:B:115:ILE:N	2.59	0.55
1:E:3:PHE:O	1:E:48:THR:N	2.37	0.55
1:A:154:VAL:O	1:A:158:LEU:HD21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HG12	1:B:5:VAL:O	2.06	0.55
1:F:21:ALA:O	1:F:22:ALA:C	2.44	0.55
1:F:82:PRO:O	1:F:83:ARG:C	2.45	0.55
1:H:125:LEU:HG	1:H:125:LEU:O	2.05	0.55
1:G:61:GLY:O	1:G:62:PHE:CG	2.59	0.55
1:G:155:VAL:CA	1:G:158:LEU:HD23	2.36	0.55
1:F:167:GLN:CA	1:F:167:GLN:HE21	2.16	0.55
1:E:65:ALA:O	1:E:68:ARG:N	2.40	0.55
1:F:78:SER:O	1:F:80:VAL:N	2.40	0.55
1:G:70:LEU:N	1:G:70:LEU:CD1	2.70	0.55
1:C:77:VAL:HG12	1:C:78:SER:O	2.06	0.55
1:D:191:ALA:O	1:D:192:LEU:C	2.44	0.55
1:F:191:ALA:O	1:F:192:LEU:C	2.44	0.55
1:C:54:GLU:CD	1:C:55:ASP:N	2.60	0.55
1:G:101:LEU:O	1:G:102:ALA:CB	2.54	0.55
1:A:11:GLU:HB2	1:A:18:VAL:HG22	1.89	0.55
1:F:29:ASN:H	1:F:29:ASN:HD22	1.55	0.55
1:G:67:ASN:O	1:G:68:ARG:C	2.45	0.55
1:H:167:GLN:HE21	1:H:167:GLN:CA	2.16	0.55
1:B:82:PRO:O	1:B:86:MET:HB2	2.05	0.55
1:G:110:THR:C	1:G:112:VAL:H	2.11	0.55
1:E:155:VAL:CA	1:E:158:LEU:HD23	2.35	0.55
1:G:104:SER:O	1:G:106:VAL:HG12	2.07	0.55
1:H:166:LYS:HA	1:H:169:GLU:OE2	2.06	0.55
1:G:72:LEU:O	1:G:73:ALA:C	2.45	0.54
1:F:113:PRO:C	1:F:115:ILE:N	2.59	0.54
1:C:77:VAL:C	1:C:80:VAL:HG12	2.28	0.54
1:B:112:VAL:HG23	1:B:113:PRO:O	2.07	0.54
1:H:157:ALA:O	1:H:160:GLY:N	2.39	0.54
1:G:112:VAL:CG1	1:G:113:PRO:HD2	2.36	0.54
1:F:112:VAL:HG23	1:F:113:PRO:O	2.07	0.54
1:C:86:MET:O	1:C:87:ALA:C	2.45	0.54
1:B:16:HIS:CD2	1:B:27:ARG:HD3	2.43	0.54
1:A:86:MET:O	1:A:87:ALA:C	2.45	0.54
1:D:165:ALA:O	1:D:166:LYS:C	2.43	0.54
1:B:73:ALA:O	1:B:74:LEU:C	2.43	0.54
1:G:86:MET:O	1:G:87:ALA:C	2.44	0.54
1:C:70:LEU:N	1:C:70:LEU:CD1	2.70	0.54
1:B:191:ALA:O	1:B:192:LEU:C	2.45	0.54
1:C:31:THR:C	1:C:35:LEU:HD12	2.27	0.54
1:D:78:SER:O	1:D:80:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:O	1:A:16:HIS:HB3	2.06	0.54
1:H:78:SER:O	1:H:80:VAL:N	2.41	0.54
1:A:71:PHE:HA	1:A:74:LEU:HD12	1.90	0.54
1:G:77:VAL:C	1:G:80:VAL:HG12	2.28	0.54
1:E:82:PRO:O	1:E:85:ALA:HB3	2.08	0.54
1:B:112:VAL:HG23	1:B:113:PRO:N	2.23	0.54
1:E:48:THR:HG22	1:E:61:GLY:HA2	1.90	0.54
1:B:29:ASN:HD22	1:B:29:ASN:H	1.56	0.54
1:H:16:HIS:CD2	1:H:27:ARG:HD3	2.42	0.54
1:E:54:GLU:CD	1:E:55:ASP:N	2.61	0.54
1:E:86:MET:O	1:E:87:ALA:C	2.46	0.54
1:A:189:SER:OG	1:A:190:SER:N	2.41	0.54
1:A:11:GLU:HB2	1:A:18:VAL:CG2	2.37	0.54
1:A:110:THR:C	1:A:112:VAL:H	2.11	0.54
1:A:77:VAL:C	1:A:80:VAL:HG12	2.28	0.54
1:D:94:ALA:O	1:D:95:ALA:C	2.45	0.54
1:E:4:SER:OG	1:E:5:VAL:N	2.40	0.54
1:C:11:GLU:HB2	1:C:18:VAL:HG22	1.89	0.54
1:B:78:SER:O	1:B:80:VAL:N	2.40	0.54
1:F:16:HIS:CE1	1:F:27:ARG:HD3	2.43	0.54
1:A:126:GLU:CA	1:A:126:GLU:OE1	2.50	0.54
1:E:77:VAL:C	1:E:80:VAL:HG12	2.28	0.54
1:D:167:GLN:HA	1:D:167:GLN:NE2	2.21	0.54
1:G:11:GLU:HB2	1:G:18:VAL:CG2	2.38	0.54
1:C:129:ASP:O	1:C:131:VAL:N	2.34	0.54
1:E:148:ASN:HA	1:E:151:ARG:CD	2.38	0.54
1:G:82:PRO:O	1:G:85:ALA:HB3	2.08	0.54
1:H:112:VAL:HG23	1:H:113:PRO:N	2.22	0.54
1:E:189:SER:O	1:E:192:LEU:N	2.41	0.54
1:F:167:GLN:CA	1:F:167:GLN:NE2	2.67	0.54
1:C:105:ASP:O	1:C:108:SER:N	2.41	0.54
1:G:106:VAL:O	1:G:107:ALA:C	2.45	0.54
1:G:105:ASP:O	1:G:108:SER:N	2.41	0.54
1:C:148:ASN:HA	1:C:151:ARG:CD	2.38	0.54
1:E:11:GLU:HB2	1:E:18:VAL:HG22	1.89	0.53
1:G:70:LEU:HD13	1:G:70:LEU:H	1.74	0.53
1:F:94:ALA:O	1:F:95:ALA:C	2.46	0.53
1:E:110:THR:C	1:E:112:VAL:H	2.11	0.53
1:B:16:HIS:CE1	1:B:27:ARG:HD3	2.43	0.53
1:G:148:ASN:HA	1:G:151:ARG:CD	2.38	0.53
1:H:94:ALA:O	1:H:95:ALA:C	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:O	1:A:195:ALA:N	2.30	0.53
1:G:104:SER:O	1:G:106:VAL:N	2.36	0.53
1:H:70:LEU:CD2	1:H:70:LEU:N	2.65	0.53
1:A:109:LEU:O	1:A:110:THR:C	2.44	0.53
1:F:91:VAL:CG1	1:F:92:HIS:N	2.54	0.53
1:C:85:ALA:O	1:C:86:MET:C	2.44	0.53
1:B:100:ALA:O	1:B:104:SER:N	2.41	0.53
1:C:189:SER:OG	1:C:190:SER:N	2.41	0.53
1:G:11:GLU:HB2	1:G:18:VAL:HG22	1.90	0.53
1:A:70:LEU:N	1:A:70:LEU:CD1	2.71	0.53
1:C:82:PRO:O	1:C:85:ALA:HB3	2.08	0.53
1:B:109:LEU:C	1:B:111:ARG:N	2.58	0.53
1:E:70:LEU:N	1:E:70:LEU:CD1	2.72	0.53
1:A:105:ASP:O	1:A:108:SER:N	2.41	0.53
1:A:4:SER:OG	1:A:5:VAL:N	2.42	0.53
1:G:189:SER:OG	1:G:190:SER:N	2.42	0.53
1:A:11:GLU:HA	1:A:11:GLU:OE1	2.09	0.53
1:C:154:VAL:HG22	1:C:188:THR:O	2.09	0.53
1:C:172:THR:HG23	1:C:173:ASP:N	2.19	0.53
1:E:67:ASN:O	1:E:68:ARG:C	2.46	0.53
1:A:35:LEU:H	1:A:35:LEU:HD12	1.74	0.53
1:C:15:ASP:O	1:C:16:HIS:HB3	2.07	0.53
1:E:11:GLU:HA	1:E:11:GLU:OE1	2.09	0.53
1:F:100:ALA:O	1:F:104:SER:N	2.42	0.53
1:H:16:HIS:CE1	1:H:27:ARG:HD3	2.44	0.53
1:C:35:LEU:HD12	1:C:35:LEU:H	1.73	0.53
1:F:112:VAL:HG23	1:F:113:PRO:N	2.23	0.53
1:D:100:ALA:O	1:D:104:SER:N	2.42	0.53
1:A:155:VAL:CA	1:A:158:LEU:HD23	2.36	0.53
1:E:172:THR:HG23	1:E:173:ASP:N	2.18	0.53
1:C:115:ILE:O	1:C:115:ILE:CG2	2.54	0.53
1:G:102:ALA:C	1:G:104:SER:N	2.62	0.53
1:C:126:GLU:OE1	1:C:126:GLU:CA	2.50	0.53
1:D:130:LYS:O	1:D:131:VAL:CB	2.47	0.53
1:E:106:VAL:O	1:E:107:ALA:C	2.45	0.53
1:A:102:ALA:C	1:A:104:SER:N	2.62	0.53
1:D:73:ALA:O	1:D:76:SER:N	2.42	0.53
1:E:11:GLU:HB2	1:E:18:VAL:CG2	2.39	0.53
1:F:97:LEU:O	1:F:99:GLN:N	2.42	0.53
1:A:152:GLY:O	1:A:156:GLU:HB2	2.09	0.53
1:A:189:SER:O	1:A:192:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ARG:NH1	1:F:193:ARG:HG3	2.23	0.53
1:F:202:THR:HG22	1:F:203:ARG:NH2	2.24	0.53
1:B:82:PRO:O	1:B:83:ARG:C	2.46	0.52
1:C:67:ASN:O	1:C:68:ARG:C	2.47	0.52
1:E:154:VAL:HG22	1:E:188:THR:O	2.09	0.52
1:E:189:SER:OG	1:E:190:SER:N	2.41	0.52
1:G:189:SER:O	1:G:192:LEU:N	2.42	0.52
1:C:110:THR:C	1:C:112:VAL:H	2.11	0.52
1:D:82:PRO:O	1:D:83:ARG:C	2.45	0.52
1:C:193:ARG:HA	1:C:196:LEU:HD21	1.91	0.52
1:G:172:THR:HG23	1:G:173:ASP:N	2.19	0.52
1:G:154:VAL:HG22	1:G:188:THR:O	2.10	0.52
1:B:170:GLU:O	1:B:171:ALA:HB2	2.09	0.52
1:G:77:VAL:CG1	1:G:78:SER:N	2.72	0.52
1:G:82:PRO:O	1:G:83:ARG:C	2.47	0.52
1:C:102:ALA:C	1:C:104:SER:N	2.63	0.52
1:A:148:ASN:HA	1:A:151:ARG:CD	2.40	0.52
1:C:11:GLU:HB2	1:C:18:VAL:CG2	2.39	0.52
1:D:16:HIS:CE1	1:D:27:ARG:HD3	2.44	0.52
1:H:193:ARG:HG3	1:H:193:ARG:NH1	2.23	0.52
1:H:155:VAL:CG1	1:H:156:GLU:N	2.73	0.52
1:G:8:GLU:HG2	1:G:8:GLU:O	2.10	0.52
1:H:118:ARG:HB2	1:H:118:ARG:NH1	2.25	0.52
1:F:105:ASP:OD1	1:F:106:VAL:N	2.42	0.52
1:E:115:ILE:O	1:E:115:ILE:CG2	2.54	0.52
1:B:94:ALA:O	1:B:95:ALA:C	2.46	0.52
1:H:100:ALA:O	1:H:104:SER:N	2.42	0.52
1:D:202:THR:HG22	1:D:203:ARG:NH2	2.25	0.52
1:D:46:LEU:HD12	1:D:47:VAL:O	2.09	0.52
1:F:83:ARG:HB2	1:F:84:LEU:CD1	2.29	0.52
1:A:88:THR:O	1:A:92:HIS:N	2.42	0.52
1:B:97:LEU:O	1:B:99:GLN:N	2.43	0.52
1:H:105:ASP:OD1	1:H:106:VAL:N	2.43	0.52
1:B:46:LEU:HD12	1:B:47:VAL:O	2.10	0.52
1:F:118:ARG:NH1	1:F:118:ARG:HB2	2.25	0.52
1:H:73:ALA:O	1:H:76:SER:N	2.42	0.52
1:A:82:PRO:O	1:A:83:ARG:C	2.46	0.52
1:C:88:THR:O	1:C:92:HIS:N	2.43	0.52
1:D:191:ALA:O	1:D:193:ARG:N	2.43	0.52
1:D:83:ARG:HB2	1:D:84:LEU:CD1	2.29	0.52
1:H:82:PRO:O	1:H:83:ARG:C	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:PRO:O	1:H:83:ARG:O	2.28	0.52
1:C:70:LEU:HD13	1:C:70:LEU:H	1.74	0.52
1:G:11:GLU:HA	1:G:11:GLU:OE1	2.10	0.52
1:F:73:ALA:O	1:F:76:SER:N	2.43	0.52
1:G:88:THR:O	1:G:92:HIS:N	2.43	0.52
1:E:82:PRO:O	1:E:83:ARG:C	2.49	0.52
1:D:105:ASP:OD1	1:D:106:VAL:N	2.43	0.52
1:C:189:SER:O	1:C:192:LEU:N	2.43	0.52
1:D:170:GLU:O	1:D:171:ALA:HB2	2.09	0.52
1:G:35:LEU:HD12	1:G:35:LEU:H	1.75	0.52
1:H:91:VAL:CG1	1:H:92:HIS:N	2.54	0.52
1:G:4:SER:OG	1:G:5:VAL:N	2.41	0.52
1:D:14:LEU:N	1:D:14:LEU:HD12	2.14	0.52
1:D:149:ALA:O	1:D:152:GLY:N	2.42	0.52
1:D:82:PRO:O	1:D:83:ARG:O	2.28	0.51
1:B:73:ALA:O	1:B:76:SER:N	2.42	0.51
1:G:189:SER:O	1:G:190:SER:C	2.49	0.51
1:F:149:ALA:O	1:F:152:GLY:N	2.42	0.51
1:A:77:VAL:HG12	1:A:78:SER:H	1.76	0.51
1:A:82:PRO:O	1:A:85:ALA:HB3	2.09	0.51
1:H:97:LEU:O	1:H:99:GLN:N	2.42	0.51
1:G:94:ALA:O	1:G:98:ARG:N	2.41	0.51
1:D:105:ASP:OD1	1:D:107:ALA:N	2.43	0.51
1:E:193:ARG:HA	1:E:196:LEU:HD21	1.92	0.51
1:D:198:LEU:HD23	1:D:198:LEU:C	2.31	0.51
1:D:152:GLY:O	1:D:153:SER:C	2.49	0.51
1:F:105:ASP:OD1	1:F:107:ALA:N	2.43	0.51
1:E:84:LEU:O	1:E:85:ALA:C	2.49	0.51
1:A:189:SER:C	1:A:191:ALA:N	2.61	0.51
1:B:156:GLU:OE1	1:B:156:GLU:O	2.28	0.51
1:E:7:GLY:HA3	1:E:19:ILE:HG22	1.93	0.51
1:G:2:ILE:HB	1:G:50:MET:HE2	1.92	0.51
1:H:152:GLY:O	1:H:153:SER:C	2.49	0.51
1:C:11:GLU:OE1	1:C:11:GLU:HA	2.10	0.51
1:E:189:SER:O	1:E:190:SER:C	2.49	0.51
1:C:189:SER:C	1:C:191:ALA:N	2.62	0.51
1:B:198:LEU:C	1:B:200:GLY:H	2.14	0.51
1:H:202:THR:HG22	1:H:203:ARG:NH2	2.25	0.51
1:B:168:ALA:O	1:B:171:ALA:HB3	2.10	0.51
1:G:94:ALA:O	1:G:97:LEU:HB3	2.11	0.51
1:E:105:ASP:O	1:E:108:SER:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:GLU:O	1:F:171:ALA:HB2	2.11	0.51
1:B:43:GLN:O	1:B:44:ALA:HB2	2.11	0.51
1:E:77:VAL:CG1	1:E:78:SER:N	2.73	0.51
1:C:4:SER:OG	1:C:5:VAL:N	2.41	0.51
1:F:191:ALA:O	1:F:193:ARG:N	2.43	0.51
1:H:170:GLU:O	1:H:171:ALA:HB2	2.10	0.51
1:C:77:VAL:HG12	1:C:78:SER:H	1.76	0.51
1:H:117:ARG:O	1:H:118:ARG:C	2.49	0.51
1:C:82:PRO:O	1:C:83:ARG:C	2.48	0.51
1:B:108:SER:HA	1:C:202:THR:HB	1.93	0.51
1:C:129:ASP:C	1:C:131:VAL:H	2.13	0.51
1:G:193:ARG:HA	1:G:196:LEU:HD21	1.93	0.51
1:H:155:VAL:O	1:H:156:GLU:C	2.50	0.51
1:G:166:LYS:H	1:G:166:LYS:CD	2.24	0.51
1:A:24:ILE:HD12	1:B:21:ALA:HB1	1.93	0.51
1:A:202:THR:HB	1:D:108:SER:HA	1.92	0.51
1:B:105:ASP:OD1	1:B:106:VAL:N	2.44	0.51
1:G:158:LEU:HA	1:G:161:LEU:HD12	1.93	0.51
1:F:152:GLY:O	1:F:153:SER:C	2.48	0.51
1:H:149:ALA:O	1:H:152:GLY:N	2.42	0.51
1:B:149:ALA:O	1:B:152:GLY:N	2.42	0.51
1:E:88:THR:O	1:E:92:HIS:N	2.43	0.51
1:D:127:LEU:HD22	1:D:131:VAL:HG23	1.93	0.51
1:A:189:SER:O	1:A:190:SER:C	2.49	0.51
1:A:193:ARG:HA	1:A:196:LEU:HD21	1.92	0.51
1:D:156:GLU:O	1:D:156:GLU:OE1	2.29	0.51
1:E:70:LEU:HD13	1:E:70:LEU:H	1.76	0.51
1:A:94:ALA:O	1:A:98:ARG:N	2.41	0.51
1:B:118:ARG:NH1	1:B:118:ARG:HB2	2.26	0.51
1:D:118:ARG:NH1	1:D:118:ARG:HB2	2.26	0.51
1:A:154:VAL:HG22	1:A:188:THR:O	2.10	0.50
1:C:152:GLY:O	1:C:156:GLU:HB2	2.12	0.50
1:G:152:GLY:O	1:G:156:GLU:HB2	2.10	0.50
1:B:202:THR:HG22	1:B:203:ARG:NH2	2.27	0.50
1:A:166:LYS:H	1:A:166:LYS:CD	2.24	0.50
1:H:118:ARG:O	1:H:121:GLU:HB2	2.12	0.50
1:F:82:PRO:O	1:F:83:ARG:O	2.29	0.50
1:A:70:LEU:H	1:A:70:LEU:HD13	1.75	0.50
1:B:105:ASP:OD1	1:B:107:ALA:N	2.45	0.50
1:G:129:ASP:C	1:G:131:VAL:H	2.13	0.50
1:B:191:ALA:O	1:B:193:ARG:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ALA:O	1:E:97:LEU:HB3	2.12	0.50
1:A:105:ASP:O	1:A:106:VAL:C	2.49	0.50
1:D:46:LEU:HD11	1:D:61:GLY:HA3	1.94	0.50
1:F:118:ARG:O	1:F:121:GLU:HB2	2.11	0.50
1:D:117:ARG:O	1:D:118:ARG:C	2.49	0.50
1:C:8:GLU:HG2	1:C:10:LEU:HD23	1.93	0.50
1:E:8:GLU:HG2	1:E:10:LEU:HD23	1.93	0.50
1:F:15:ASP:O	1:F:35:LEU:HD21	2.12	0.50
1:D:91:VAL:CG1	1:D:92:HIS:N	2.53	0.50
1:D:97:LEU:O	1:D:99:GLN:N	2.44	0.50
1:C:189:SER:O	1:C:190:SER:C	2.49	0.50
1:D:200:GLY:O	1:D:201:LYS:C	2.50	0.50
1:C:104:SER:O	1:C:106:VAL:N	2.35	0.50
1:E:102:ALA:C	1:E:104:SER:N	2.63	0.50
1:B:118:ARG:O	1:B:121:GLU:HB2	2.11	0.50
1:G:119:GLY:O	1:G:120:ALA:C	2.50	0.50
1:A:163:PHE:CE1	1:D:113:PRO:HD3	2.47	0.50
1:B:91:VAL:CG1	1:B:92:HIS:N	2.54	0.50
1:B:193:ARG:CG	1:B:193:ARG:HH11	2.24	0.50
1:E:106:VAL:HG22	1:E:107:ALA:N	2.26	0.50
1:F:173:ASP:C	1:F:175:VAL:N	2.64	0.50
1:F:112:VAL:HA	1:G:163:PHE:CE1	2.41	0.50
1:C:110:THR:C	1:C:112:VAL:N	2.65	0.50
1:F:201:LYS:HG2	1:F:202:THR:N	2.27	0.50
1:F:155:VAL:O	1:F:156:GLU:C	2.50	0.50
1:H:165:ALA:C	1:H:167:GLN:N	2.63	0.50
1:H:46:LEU:HD12	1:H:47:VAL:O	2.12	0.50
1:E:24:ILE:HD12	1:F:21:ALA:HB1	1.93	0.50
1:A:110:THR:C	1:A:112:VAL:N	2.65	0.50
1:B:130:LYS:O	1:B:131:VAL:CB	2.47	0.50
1:E:152:GLY:O	1:E:156:GLU:HB2	2.11	0.50
1:B:201:LYS:HG2	1:B:202:THR:N	2.26	0.50
1:H:168:ALA:O	1:H:171:ALA:HB3	2.11	0.50
1:D:168:ALA:O	1:D:171:ALA:HB3	2.12	0.50
1:C:7:GLY:HA3	1:C:19:ILE:HG22	1.94	0.50
1:C:10:LEU:HB2	1:C:18:VAL:HG23	1.94	0.50
1:A:112:VAL:CG1	1:A:115:ILE:HG13	2.42	0.50
1:A:77:VAL:CG1	1:A:78:SER:N	2.73	0.50
1:F:108:SER:O	1:F:111:ARG:CB	2.60	0.50
1:F:127:LEU:HD22	1:F:131:VAL:HG23	1.92	0.50
1:H:105:ASP:OD1	1:H:107:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:LEU:HD22	1:H:131:VAL:HG23	1.93	0.50
1:F:46:LEU:HD12	1:F:47:VAL:O	2.12	0.50
1:E:10:LEU:HB2	1:E:18:VAL:HG23	1.93	0.50
1:H:108:SER:O	1:H:111:ARG:CB	2.60	0.50
1:E:129:ASP:C	1:E:131:VAL:H	2.14	0.50
1:A:173:ASP:HA	1:A:176:LEU:HB3	1.93	0.50
1:E:166:LYS:CD	1:E:166:LYS:H	2.24	0.50
1:E:35:LEU:HD12	1:E:35:LEU:H	1.74	0.50
1:B:152:GLY:O	1:B:153:SER:C	2.50	0.50
1:E:8:GLU:HG2	1:E:8:GLU:O	2.11	0.50
1:D:108:SER:O	1:D:111:ARG:CB	2.60	0.50
1:G:5:VAL:O	1:G:5:VAL:CG1	2.54	0.50
1:A:127:LEU:O	1:A:128:ALA:HB3	2.11	0.50
1:H:191:ALA:O	1:H:193:ARG:N	2.45	0.50
1:G:192:LEU:O	1:G:195:ALA:N	2.31	0.50
1:F:165:ALA:C	1:F:167:GLN:N	2.63	0.50
1:A:94:ALA:O	1:A:97:LEU:HB3	2.11	0.50
1:C:166:LYS:CD	1:C:166:LYS:H	2.24	0.50
1:C:16:HIS:ND1	1:C:27:ARG:CZ	2.75	0.49
1:C:16:HIS:CG	1:C:27:ARG:NH2	2.80	0.49
1:C:24:ILE:HD12	1:D:21:ALA:HB1	1.94	0.49
1:C:84:LEU:O	1:C:85:ALA:C	2.51	0.49
1:E:110:THR:C	1:E:112:VAL:N	2.65	0.49
1:E:112:VAL:CG1	1:E:115:ILE:HG13	2.42	0.49
1:D:107:ALA:O	1:D:108:SER:C	2.51	0.49
1:B:127:LEU:HD22	1:B:131:VAL:HG23	1.93	0.49
1:D:193:ARG:HH11	1:D:193:ARG:CG	2.24	0.49
1:F:117:ARG:O	1:F:118:ARG:C	2.49	0.49
1:C:119:GLY:O	1:C:120:ALA:C	2.50	0.49
1:A:16:HIS:CG	1:A:27:ARG:NH2	2.80	0.49
1:F:108:SER:HA	1:G:202:THR:HB	1.94	0.49
1:C:5:VAL:O	1:C:5:VAL:CG1	2.54	0.49
1:H:156:GLU:O	1:H:156:GLU:OE1	2.30	0.49
1:E:94:ALA:O	1:E:98:ARG:N	2.42	0.49
1:H:43:GLN:O	1:H:44:ALA:HB2	2.12	0.49
1:A:8:GLU:HG2	1:A:10:LEU:HD23	1.94	0.49
1:B:68:ARG:CG	1:B:69:ASP:N	2.75	0.49
1:H:2:ILE:O	1:H:3:PHE:HD1	1.95	0.49
1:F:131:VAL:HG13	1:F:132:GLY:N	2.28	0.49
1:E:158:LEU:HA	1:E:161:LEU:HD12	1.94	0.49
1:C:105:ASP:O	1:C:106:VAL:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ASP:O	1:E:72:LEU:HB2	2.12	0.49
1:H:173:ASP:C	1:H:175:VAL:N	2.65	0.49
1:G:84:LEU:O	1:G:85:ALA:C	2.51	0.49
1:F:107:ALA:O	1:F:108:SER:C	2.50	0.49
1:B:108:SER:O	1:B:111:ARG:CB	2.60	0.49
1:H:107:ALA:O	1:H:108:SER:C	2.51	0.49
1:H:131:VAL:HG13	1:H:132:GLY:N	2.28	0.49
1:B:200:GLY:O	1:B:201:LYS:C	2.50	0.49
1:H:200:GLY:O	1:H:201:LYS:C	2.50	0.49
1:G:105:ASP:O	1:G:106:VAL:C	2.50	0.49
1:F:168:ALA:O	1:F:171:ALA:HB3	2.12	0.49
1:F:46:LEU:HD11	1:F:61:GLY:HA3	1.94	0.49
1:E:119:GLY:O	1:E:120:ALA:C	2.51	0.49
1:C:8:GLU:HG2	1:C:8:GLU:O	2.11	0.49
1:D:31:THR:CB	1:D:32:PRO:HD2	2.42	0.49
1:B:82:PRO:O	1:B:83:ARG:O	2.30	0.49
1:G:16:HIS:CG	1:G:27:ARG:NH2	2.80	0.49
1:F:14:LEU:N	1:F:14:LEU:HD12	2.13	0.49
1:F:200:GLY:O	1:F:201:LYS:C	2.50	0.49
1:F:156:GLU:O	1:F:156:GLU:OE1	2.30	0.49
1:D:118:ARG:O	1:D:121:GLU:HB2	2.12	0.49
1:B:198:LEU:C	1:B:198:LEU:HD23	2.33	0.49
1:E:173:ASP:HA	1:E:176:LEU:HB3	1.94	0.49
1:H:201:LYS:HG2	1:H:202:THR:N	2.26	0.49
1:D:198:LEU:C	1:D:200:GLY:H	2.16	0.49
1:G:31:THR:O	1:G:35:LEU:HD12	2.13	0.49
1:H:83:ARG:HB2	1:H:84:LEU:CD1	2.30	0.49
1:C:94:ALA:O	1:C:97:LEU:HB3	2.12	0.49
1:B:117:ARG:O	1:B:118:ARG:C	2.49	0.49
1:D:15:ASP:O	1:D:35:LEU:HD21	2.11	0.49
1:B:83:ARG:HB2	1:B:84:LEU:CD1	2.29	0.49
1:A:158:LEU:HA	1:A:161:LEU:HD12	1.94	0.49
1:E:192:LEU:O	1:E:192:LEU:HD13	2.13	0.49
1:G:11:GLU:N	1:G:18:VAL:CG2	2.76	0.49
1:B:31:THR:CB	1:B:32:PRO:HD2	2.43	0.49
1:H:31:THR:CB	1:H:32:PRO:HD2	2.43	0.49
1:G:77:VAL:HG12	1:G:78:SER:H	1.74	0.49
1:D:105:ASP:O	1:D:106:VAL:HB	2.13	0.49
1:C:127:LEU:O	1:C:128:ALA:HB3	2.13	0.49
1:C:173:ASP:HA	1:C:176:LEU:HB3	1.94	0.49
1:B:165:ALA:C	1:B:167:GLN:N	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLU:N	1:C:18:VAL:CG2	2.76	0.48
1:F:31:THR:CB	1:F:32:PRO:HD2	2.43	0.48
1:H:15:ASP:O	1:H:35:LEU:HD21	2.13	0.48
1:G:112:VAL:HB	1:G:115:ILE:HG13	1.95	0.48
1:C:158:LEU:HA	1:C:161:LEU:HD12	1.93	0.48
1:H:46:LEU:HD11	1:H:61:GLY:HA3	1.95	0.48
1:D:173:ASP:C	1:D:175:VAL:N	2.66	0.48
1:G:8:GLU:HG2	1:G:10:LEU:HD23	1.93	0.48
1:G:24:ILE:HD12	1:H:21:ALA:HB1	1.94	0.48
1:H:48:THR:HG23	1:H:49:ALA:H	1.76	0.48
1:H:71:PHE:O	1:H:72:LEU:C	2.52	0.48
1:G:112:VAL:CG1	1:G:115:ILE:HG13	2.43	0.48
1:F:119:GLY:O	1:F:120:ALA:C	2.52	0.48
1:D:155:VAL:O	1:D:156:GLU:C	2.51	0.48
1:A:16:HIS:ND1	1:A:27:ARG:CZ	2.76	0.48
1:F:16:HIS:NE2	1:F:27:ARG:HD3	2.29	0.48
1:C:69:ASP:O	1:C:72:LEU:HB2	2.13	0.48
1:E:112:VAL:HB	1:E:115:ILE:HG13	1.96	0.48
1:H:193:ARG:CG	1:H:193:ARG:HH11	2.26	0.48
1:H:198:LEU:C	1:H:200:GLY:H	2.16	0.48
1:A:106:VAL:HG22	1:A:107:ALA:N	2.26	0.48
1:F:193:ARG:CG	1:F:193:ARG:HH11	2.26	0.48
1:B:198:LEU:C	1:B:200:GLY:N	2.66	0.48
1:A:53:ARG:O	1:A:54:GLU:C	2.52	0.48
1:G:7:GLY:HA3	1:G:19:ILE:HG22	1.95	0.48
1:H:80:VAL:O	1:H:83:ARG:HG3	2.14	0.48
1:A:163:PHE:N	1:D:113:PRO:HG3	2.27	0.48
1:B:105:ASP:O	1:B:106:VAL:HB	2.13	0.48
1:E:127:LEU:O	1:E:128:ALA:HB3	2.13	0.48
1:H:198:LEU:HD23	1:H:198:LEU:C	2.33	0.48
1:B:155:VAL:O	1:B:156:GLU:C	2.51	0.48
1:E:31:THR:O	1:E:35:LEU:HD12	2.14	0.48
1:D:43:GLN:O	1:D:44:ALA:HB2	2.12	0.48
1:E:11:GLU:N	1:E:18:VAL:CG2	2.77	0.48
1:A:112:VAL:HB	1:A:115:ILE:HG13	1.95	0.48
1:B:112:VAL:HA	1:C:163:PHE:CE1	2.42	0.48
1:A:129:ASP:C	1:A:131:VAL:H	2.14	0.48
1:D:193:ARG:HG3	1:D:193:ARG:HH11	1.79	0.48
1:D:165:ALA:C	1:D:167:GLN:N	2.64	0.48
1:D:3:PHE:CD2	1:D:68:ARG:NH2	2.82	0.48
1:E:16:HIS:ND1	1:E:27:ARG:CZ	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:THR:HG23	1:F:49:ALA:H	1.77	0.48
1:B:131:VAL:HG13	1:B:132:GLY:N	2.27	0.48
1:G:173:ASP:HA	1:G:176:LEU:HB3	1.94	0.48
1:C:96:ALA:O	1:C:97:LEU:C	2.51	0.48
1:A:7:GLY:HA3	1:A:19:ILE:HG22	1.96	0.48
1:A:11:GLU:N	1:A:18:VAL:CG2	2.76	0.48
1:G:16:HIS:ND1	1:G:27:ARG:CZ	2.76	0.48
1:A:89:LEU:HA	1:A:92:HIS:O	2.14	0.48
1:G:70:LEU:H	1:G:70:LEU:CD1	2.26	0.48
1:G:69:ASP:O	1:G:72:LEU:HB2	2.13	0.48
1:B:173:ASP:C	1:B:175:VAL:N	2.65	0.48
1:G:106:VAL:HG22	1:G:107:ALA:N	2.27	0.48
1:B:3:PHE:CD2	1:B:68:ARG:NH2	2.82	0.48
1:F:15:ASP:N	1:F:15:ASP:OD1	2.24	0.48
1:C:30:ALA:HA	1:C:86:MET:CE	2.44	0.48
1:D:131:VAL:HG13	1:D:132:GLY:N	2.28	0.48
1:H:14:LEU:H	1:H:14:LEU:CD1	2.09	0.48
1:A:8:GLU:HG2	1:A:8:GLU:O	2.13	0.48
1:F:71:PHE:CE1	1:F:85:ALA:HB1	2.49	0.48
1:F:105:ASP:O	1:F:106:VAL:HB	2.14	0.48
1:F:198:LEU:HD23	1:F:198:LEU:C	2.33	0.48
1:F:198:LEU:C	1:F:200:GLY:H	2.16	0.48
1:C:31:THR:O	1:C:35:LEU:HD12	2.14	0.48
1:F:72:LEU:HD23	1:F:72:LEU:HA	1.51	0.47
1:D:127:LEU:O	1:D:128:ALA:C	2.52	0.47
1:C:112:VAL:CG1	1:C:115:ILE:HG13	2.43	0.47
1:H:157:ALA:O	1:H:158:LEU:C	2.52	0.47
1:D:167:GLN:CA	1:D:167:GLN:HE21	2.16	0.47
1:A:31:THR:O	1:A:35:LEU:HD12	2.13	0.47
1:F:80:VAL:O	1:F:83:ARG:HG3	2.14	0.47
1:A:84:LEU:O	1:A:85:ALA:C	2.51	0.47
1:C:70:LEU:CD1	1:C:70:LEU:H	2.26	0.47
1:D:106:VAL:O	1:D:109:LEU:HB2	2.14	0.47
1:E:6:ARG:HG3	1:E:45:ARG:CB	2.40	0.47
1:D:192:LEU:C	1:D:194:ALA:N	2.68	0.47
1:C:192:LEU:HD13	1:C:192:LEU:O	2.14	0.47
1:F:157:ALA:O	1:F:158:LEU:C	2.51	0.47
1:A:119:GLY:O	1:A:120:ALA:C	2.50	0.47
1:B:15:ASP:O	1:B:35:LEU:HD21	2.15	0.47
1:B:2:ILE:O	1:B:3:PHE:HD1	1.97	0.47
1:E:16:HIS:CG	1:E:27:ARG:NH2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:LEU:O	1:G:128:ALA:HB3	2.13	0.47
1:C:153:SER:O	1:C:155:VAL:N	2.48	0.47
1:B:156:GLU:O	1:B:157:ALA:C	2.53	0.47
1:D:201:LYS:HG2	1:D:202:THR:N	2.27	0.47
1:A:84:LEU:O	1:A:87:ALA:HB3	2.14	0.47
1:G:110:THR:C	1:G:112:VAL:N	2.65	0.47
1:C:77:VAL:CG1	1:C:78:SER:N	2.73	0.47
1:H:105:ASP:O	1:H:106:VAL:HB	2.14	0.47
1:G:53:ARG:O	1:G:54:GLU:C	2.52	0.47
1:E:96:ALA:O	1:E:97:LEU:C	2.51	0.47
1:H:171:ALA:O	1:H:175:VAL:HG23	2.14	0.47
1:A:69:ASP:O	1:A:72:LEU:HB2	2.15	0.47
1:F:113:PRO:HD3	1:G:163:PHE:CE1	2.50	0.47
1:E:77:VAL:HG12	1:E:78:SER:H	1.77	0.47
1:H:16:HIS:NE2	1:H:27:ARG:HD3	2.30	0.47
1:C:112:VAL:HB	1:C:115:ILE:HG13	1.97	0.47
1:H:198:LEU:C	1:H:200:GLY:N	2.67	0.47
1:D:157:ALA:O	1:D:158:LEU:C	2.52	0.47
1:D:198:LEU:C	1:D:200:GLY:N	2.68	0.47
1:C:53:ARG:O	1:C:54:GLU:C	2.53	0.47
1:G:96:ALA:O	1:G:97:LEU:C	2.51	0.47
1:B:46:LEU:HD11	1:B:61:GLY:HA3	1.95	0.47
1:D:68:ARG:CG	1:D:69:ASP:N	2.76	0.47
1:F:68:ARG:CG	1:F:69:ASP:N	2.76	0.47
1:A:112:VAL:HG12	1:A:113:PRO:O	2.14	0.47
1:E:30:ALA:HA	1:E:86:MET:CE	2.44	0.47
1:B:113:PRO:HD3	1:C:163:PHE:CE1	2.50	0.47
1:D:16:HIS:NE2	1:D:27:ARG:HD3	2.29	0.47
1:H:154:VAL:O	1:H:157:ALA:N	2.48	0.47
1:E:105:ASP:O	1:E:106:VAL:C	2.51	0.47
1:D:71:PHE:CE1	1:D:85:ALA:HB1	2.50	0.47
1:B:71:PHE:CE1	1:B:85:ALA:HB1	2.49	0.47
1:F:3:PHE:CD2	1:F:68:ARG:NH2	2.83	0.47
1:A:110:THR:HA	1:A:115:ILE:CG2	2.45	0.47
1:A:112:VAL:C	1:A:115:ILE:HB	2.34	0.47
1:H:127:LEU:O	1:H:128:ALA:C	2.53	0.47
1:H:192:LEU:C	1:H:194:ALA:N	2.67	0.47
1:B:193:ARG:HG3	1:B:193:ARG:HH11	1.79	0.47
1:G:189:SER:C	1:G:191:ALA:N	2.62	0.47
1:D:156:GLU:O	1:D:157:ALA:C	2.53	0.47
1:C:106:VAL:HG22	1:C:107:ALA:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ALA:O	1:C:98:ARG:N	2.42	0.47
1:H:119:GLY:O	1:H:120:ALA:C	2.53	0.47
1:G:10:LEU:HB2	1:G:18:VAL:HG23	1.95	0.47
1:B:80:VAL:O	1:B:83:ARG:HG3	2.14	0.47
1:B:107:ALA:O	1:B:108:SER:C	2.52	0.47
1:A:5:VAL:CG1	1:A:5:VAL:O	2.54	0.47
1:B:157:ALA:O	1:B:158:LEU:C	2.50	0.47
1:G:30:ALA:HA	1:G:86:MET:CE	2.45	0.47
1:H:102:ALA:C	1:H:104:SER:H	2.18	0.47
1:A:153:SER:O	1:A:155:VAL:N	2.48	0.47
1:A:192:LEU:C	1:A:194:ALA:N	2.68	0.47
1:F:156:GLU:O	1:F:157:ALA:C	2.52	0.47
1:H:3:PHE:CD2	1:H:68:ARG:NH2	2.83	0.47
1:H:68:ARG:CG	1:H:69:ASP:N	2.75	0.47
1:B:192:LEU:C	1:B:194:ALA:N	2.68	0.47
1:F:192:LEU:C	1:F:194:ALA:N	2.67	0.47
1:G:192:LEU:O	1:G:192:LEU:HD13	2.15	0.47
1:A:10:LEU:HB2	1:A:18:VAL:HG23	1.97	0.46
1:G:65:ALA:O	1:G:67:ASN:N	2.48	0.46
1:A:163:PHE:CE1	1:D:112:VAL:HA	2.39	0.46
1:B:102:ALA:C	1:B:104:SER:H	2.18	0.46
1:F:198:LEU:C	1:F:200:GLY:N	2.68	0.46
1:D:154:VAL:O	1:D:157:ALA:N	2.48	0.46
1:C:94:ALA:O	1:C:95:ALA:C	2.54	0.46
1:E:104:SER:O	1:E:106:VAL:N	2.36	0.46
1:F:106:VAL:O	1:F:109:LEU:HB2	2.16	0.46
1:E:112:VAL:HG12	1:E:113:PRO:O	2.14	0.46
1:A:192:LEU:HD13	1:A:192:LEU:O	2.16	0.46
1:C:192:LEU:C	1:C:194:ALA:N	2.68	0.46
1:E:53:ARG:O	1:E:54:GLU:C	2.53	0.46
1:D:171:ALA:O	1:D:175:VAL:HG23	2.14	0.46
1:C:164:ALA:HB1	1:C:166:LYS:HD2	1.97	0.46
1:E:28:VAL:CG1	1:E:28:VAL:O	2.61	0.46
1:F:43:GLN:O	1:F:44:ALA:HB2	2.13	0.46
1:D:71:PHE:O	1:D:72:LEU:C	2.52	0.46
1:A:65:ALA:O	1:A:67:ASN:N	2.49	0.46
1:G:110:THR:HA	1:G:115:ILE:CG2	2.44	0.46
1:G:112:VAL:CG1	1:G:113:PRO:CD	2.94	0.46
1:F:127:LEU:O	1:F:128:ALA:C	2.54	0.46
1:G:45:ARG:HG3	1:G:46:LEU:N	2.30	0.46
1:A:172:THR:HG23	1:A:173:ASP:N	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:VAL:O	1:F:157:ALA:N	2.49	0.46
1:G:97:LEU:O	1:G:101:LEU:HD22	2.15	0.46
1:G:95:ALA:O	1:G:99:GLN:N	2.26	0.46
1:F:171:ALA:O	1:F:175:VAL:HG23	2.14	0.46
1:D:2:ILE:O	1:D:3:PHE:HD1	1.98	0.46
1:B:71:PHE:O	1:B:72:LEU:C	2.52	0.46
1:F:18:VAL:C	1:F:19:ILE:HG12	2.34	0.46
1:A:70:LEU:H	1:A:70:LEU:CD1	2.28	0.46
1:G:112:VAL:HG12	1:G:113:PRO:O	2.15	0.46
1:G:112:VAL:C	1:G:115:ILE:HB	2.34	0.46
1:C:70:LEU:CA	1:C:73:ALA:HB3	2.45	0.46
1:E:192:LEU:C	1:E:194:ALA:N	2.68	0.46
1:G:153:SER:O	1:G:155:VAL:N	2.47	0.46
1:C:97:LEU:O	1:C:101:LEU:HD22	2.16	0.46
1:A:95:ALA:O	1:A:99:GLN:N	2.27	0.46
1:D:119:GLY:O	1:D:120:ALA:C	2.52	0.46
1:B:18:VAL:C	1:B:19:ILE:HG12	2.35	0.46
1:F:71:PHE:O	1:F:72:LEU:C	2.52	0.46
1:A:30:ALA:HA	1:A:86:MET:CE	2.45	0.46
1:C:65:ALA:O	1:C:67:ASN:N	2.49	0.46
1:C:77:VAL:HB	1:C:80:VAL:HG11	1.97	0.46
1:E:89:LEU:HA	1:E:92:HIS:O	2.15	0.46
1:B:127:LEU:O	1:B:128:ALA:C	2.54	0.46
1:E:153:SER:O	1:E:155:VAL:N	2.48	0.46
1:E:189:SER:C	1:E:191:ALA:N	2.61	0.46
1:A:164:ALA:HB1	1:A:166:LYS:HD2	1.98	0.46
1:H:86:MET:O	1:H:87:ALA:C	2.54	0.46
1:A:77:VAL:HB	1:A:80:VAL:HG11	1.98	0.46
1:G:68:ARG:HD2	1:G:72:LEU:HD22	1.98	0.46
1:D:102:ALA:C	1:D:104:SER:H	2.19	0.46
1:A:6:ARG:HG3	1:A:45:ARG:CB	2.41	0.46
1:F:193:ARG:HH11	1:F:193:ARG:HG3	1.80	0.46
1:G:192:LEU:C	1:G:194:ALA:N	2.68	0.46
1:G:164:ALA:HB1	1:G:166:LYS:HD2	1.97	0.46
1:E:58:THR:HG22	1:E:59:LEU:N	2.30	0.46
1:E:110:THR:HA	1:E:115:ILE:CG2	2.45	0.46
1:A:155:VAL:HG22	1:A:156:GLU:N	2.31	0.46
1:F:169:GLU:HA	1:F:172:THR:OG1	2.16	0.46
1:E:70:LEU:CD1	1:E:70:LEU:H	2.28	0.46
1:F:102:ALA:C	1:F:104:SER:H	2.19	0.46
1:F:113:PRO:HG3	1:G:163:PHE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:VAL:CG1	1:E:113:PRO:CD	2.94	0.46
1:C:6:ARG:HG3	1:C:45:ARG:CB	2.40	0.46
1:B:167:GLN:CA	1:B:167:GLN:HE21	2.15	0.46
1:C:58:THR:HG22	1:C:59:LEU:N	2.30	0.46
1:D:80:VAL:O	1:D:83:ARG:HG3	2.15	0.46
1:G:89:LEU:HA	1:G:92:HIS:O	2.15	0.46
1:C:89:LEU:HA	1:C:92:HIS:O	2.16	0.46
1:B:113:PRO:HG3	1:C:163:PHE:N	2.31	0.46
1:D:18:VAL:C	1:D:19:ILE:HG12	2.34	0.46
1:D:86:MET:O	1:D:87:ALA:C	2.54	0.46
1:F:2:ILE:O	1:F:3:PHE:HD1	1.98	0.46
1:C:68:ARG:HD2	1:C:72:LEU:HD22	1.98	0.46
1:E:202:THR:HB	1:H:108:SER:HA	1.97	0.46
1:B:16:HIS:NE2	1:B:27:ARG:HD3	2.30	0.46
1:H:193:ARG:HG3	1:H:193:ARG:HH11	1.81	0.46
1:B:171:ALA:O	1:B:175:VAL:HG23	2.16	0.46
1:G:97:LEU:O	1:G:98:ARG:C	2.55	0.46
1:G:58:THR:HG22	1:G:59:LEU:N	2.31	0.46
1:A:2:ILE:HB	1:A:50:MET:HE2	1.97	0.45
1:H:71:PHE:CE1	1:H:85:ALA:HB1	2.50	0.45
1:G:84:LEU:O	1:G:87:ALA:HB3	2.16	0.45
1:E:163:PHE:N	1:H:113:PRO:HG3	2.30	0.45
1:C:112:VAL:HG12	1:C:113:PRO:O	2.16	0.45
1:C:112:VAL:C	1:C:115:ILE:HB	2.35	0.45
1:B:119:GLY:O	1:B:120:ALA:C	2.53	0.45
1:A:112:VAL:CG1	1:A:113:PRO:CD	2.94	0.45
1:E:112:VAL:C	1:E:115:ILE:HB	2.35	0.45
1:E:163:PHE:CE1	1:H:113:PRO:HD3	2.51	0.45
1:H:156:GLU:O	1:H:157:ALA:C	2.53	0.45
1:H:169:GLU:HA	1:H:172:THR:OG1	2.15	0.45
1:A:97:LEU:O	1:A:101:LEU:HD22	2.15	0.45
1:A:28:VAL:O	1:A:28:VAL:CG1	2.64	0.45
1:D:31:THR:HB	1:D:32:PRO:HD2	1.99	0.45
1:A:70:LEU:CA	1:A:73:ALA:HB3	2.45	0.45
1:G:70:LEU:CA	1:G:73:ALA:HB3	2.45	0.45
1:E:77:VAL:HB	1:E:80:VAL:HG11	1.98	0.45
1:B:130:LYS:HG3	1:B:131:VAL:N	2.32	0.45
1:H:106:VAL:O	1:H:109:LEU:HB2	2.17	0.45
1:C:112:VAL:CG1	1:C:113:PRO:CD	2.94	0.45
1:G:149:ALA:C	1:G:151:ARG:N	2.69	0.45
1:G:31:THR:C	1:G:35:LEU:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HD2	1:A:72:LEU:HD22	1.99	0.45
1:C:45:ARG:HG3	1:C:46:LEU:N	2.31	0.45
1:D:169:GLU:HA	1:D:172:THR:OG1	2.16	0.45
1:F:52:VAL:HG22	1:F:57:MET:HG2	1.99	0.45
1:E:95:ALA:O	1:E:99:GLN:N	2.27	0.45
1:E:65:ALA:O	1:E:67:ASN:N	2.49	0.45
1:B:106:VAL:O	1:B:109:LEU:HB2	2.16	0.45
1:C:99:GLN:O	1:C:100:ALA:C	2.55	0.45
1:G:99:GLN:O	1:G:100:ALA:C	2.55	0.45
1:C:149:ALA:C	1:C:151:ARG:N	2.70	0.45
1:F:36:ALA:O	1:F:38:LEU:N	2.50	0.45
1:B:189:SER:HB2	1:B:193:ARG:NH1	2.28	0.45
1:G:154:VAL:O	1:G:158:LEU:CD2	2.65	0.45
1:C:113:PRO:HG3	1:D:163:PHE:CD1	2.52	0.45
1:G:178:GLY:O	1:G:179:GLU:HB3	2.16	0.45
1:E:68:ARG:HD2	1:E:72:LEU:HD22	1.99	0.45
1:A:99:GLN:O	1:A:100:ALA:C	2.55	0.45
1:C:28:VAL:O	1:C:28:VAL:CG1	2.63	0.45
1:G:28:VAL:CG1	1:G:28:VAL:O	2.63	0.45
1:H:108:SER:OG	1:H:109:LEU:N	2.50	0.45
1:B:154:VAL:O	1:B:157:ALA:N	2.49	0.45
1:B:169:GLU:HA	1:B:172:THR:OG1	2.17	0.45
1:H:52:VAL:HG22	1:H:57:MET:HG2	1.99	0.45
1:E:97:LEU:O	1:E:101:LEU:HD22	2.17	0.45
1:A:96:ALA:O	1:A:97:LEU:C	2.51	0.45
1:G:8:GLU:CG	1:G:8:GLU:O	2.65	0.45
1:C:8:GLU:HG2	1:C:10:LEU:CD2	2.47	0.45
1:A:45:ARG:HG3	1:A:46:LEU:N	2.31	0.45
1:B:52:VAL:HG22	1:B:57:MET:HG2	1.99	0.45
1:A:97:LEU:O	1:A:98:ARG:C	2.55	0.45
1:A:31:THR:C	1:A:35:LEU:CD1	2.86	0.45
1:D:48:THR:HG23	1:D:49:ALA:H	1.76	0.45
1:F:86:MET:O	1:F:87:ALA:C	2.55	0.45
1:E:45:ARG:HG3	1:E:46:LEU:N	2.31	0.45
1:E:149:ALA:C	1:E:151:ARG:N	2.69	0.45
1:A:50:MET:HA	1:A:58:THR:O	2.17	0.45
1:F:34:ALA:C	1:F:36:ALA:N	2.69	0.45
1:C:86:MET:O	1:C:89:LEU:N	2.50	0.45
1:C:105:ASP:CB	1:C:108:SER:OG	2.65	0.45
1:D:52:VAL:HG22	1:D:57:MET:HG2	1.99	0.45
1:F:3:PHE:HA	1:F:48:THR:CG2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:MET:O	1:G:89:LEU:N	2.50	0.44
1:H:130:LYS:HG3	1:H:131:VAL:N	2.32	0.44
1:D:29:ASN:HD22	1:D:29:ASN:N	2.14	0.44
1:C:192:LEU:O	1:C:195:ALA:N	2.31	0.44
1:H:47:VAL:HB	1:H:62:PHE:O	2.18	0.44
1:C:29:ASN:OD1	1:C:29:ASN:O	2.34	0.44
1:H:83:ARG:HG2	1:H:83:ARG:H	1.59	0.44
1:C:155:VAL:HG22	1:C:156:GLU:N	2.32	0.44
1:A:105:ASP:CB	1:A:108:SER:OG	2.65	0.44
1:H:36:ALA:O	1:H:38:LEU:N	2.49	0.44
1:C:61:GLY:C	1:C:62:PHE:CG	2.90	0.44
1:F:189:SER:HB2	1:F:193:ARG:NH1	2.27	0.44
1:C:97:LEU:O	1:C:98:ARG:C	2.56	0.44
1:E:105:ASP:CB	1:E:108:SER:OG	2.65	0.44
1:E:94:ALA:O	1:E:95:ALA:C	2.55	0.44
1:D:24:ILE:CG2	1:D:25:GLY:N	2.79	0.44
1:B:31:THR:HB	1:B:32:PRO:HD2	2.00	0.44
1:G:77:VAL:HB	1:G:80:VAL:HG11	1.98	0.44
1:C:173:ASP:O	1:C:177:ASP:OD1	2.35	0.44
1:B:169:GLU:HG2	1:B:169:GLU:H	1.55	0.44
1:A:178:GLY:O	1:A:179:GLU:CB	2.66	0.44
1:E:178:GLY:O	1:E:179:GLU:CB	2.66	0.44
1:E:97:LEU:O	1:E:98:ARG:C	2.55	0.44
1:E:70:LEU:CA	1:E:73:ALA:HB3	2.45	0.44
1:A:94:ALA:O	1:A:95:ALA:C	2.56	0.44
1:A:94:ALA:O	1:A:97:LEU:N	2.51	0.44
1:D:175:VAL:O	1:D:176:LEU:C	2.56	0.44
1:G:165:ALA:O	1:G:169:GLU:HB2	2.17	0.44
1:H:34:ALA:C	1:H:36:ALA:N	2.70	0.44
1:D:108:SER:OG	1:D:109:LEU:N	2.50	0.44
1:B:108:SER:OG	1:B:109:LEU:N	2.51	0.44
1:H:189:SER:HB2	1:H:193:ARG:NH1	2.28	0.44
1:F:189:SER:C	1:F:191:ALA:H	2.21	0.44
1:B:175:VAL:O	1:B:176:LEU:C	2.55	0.44
1:A:31:THR:O	1:A:32:PRO:C	2.55	0.44
1:C:50:MET:HA	1:C:58:THR:O	2.18	0.44
1:B:48:THR:HG23	1:B:49:ALA:H	1.76	0.44
1:D:110:THR:O	1:D:111:ARG:C	2.56	0.44
1:G:173:ASP:O	1:G:177:ASP:OD1	2.36	0.44
1:D:154:VAL:O	1:D:155:VAL:C	2.56	0.44
1:C:95:ALA:O	1:C:99:GLN:N	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ALA:O	1:C:97:LEU:N	2.50	0.44
1:G:94:ALA:O	1:G:95:ALA:C	2.56	0.44
1:H:175:VAL:O	1:H:176:LEU:C	2.55	0.44
1:C:130:LYS:HA	1:C:130:LYS:HD3	1.71	0.44
1:B:34:ALA:C	1:B:36:ALA:N	2.69	0.44
1:B:86:MET:O	1:B:87:ALA:C	2.55	0.44
1:G:163:PHE:HE2	1:G:199:LEU:HB3	1.83	0.44
1:E:86:MET:O	1:E:89:LEU:N	2.51	0.44
1:B:109:LEU:O	1:B:112:VAL:HG13	2.18	0.44
1:E:3:PHE:O	1:E:48:THR:OG1	2.30	0.44
1:H:154:VAL:O	1:H:155:VAL:C	2.56	0.44
1:G:94:ALA:O	1:G:97:LEU:N	2.51	0.44
1:E:164:ALA:HB1	1:E:166:LYS:HD2	1.99	0.44
1:E:32:PRO:O	1:E:33:SER:C	2.55	0.44
1:G:31:THR:O	1:G:32:PRO:C	2.55	0.44
1:F:121:GLU:O	1:F:122:ARG:C	2.56	0.44
1:D:121:GLU:O	1:D:122:ARG:C	2.55	0.44
1:A:120:ALA:O	1:A:121:GLU:C	2.56	0.44
1:B:24:ILE:CG2	1:B:25:GLY:N	2.80	0.44
1:H:31:THR:CA	1:H:35:LEU:HD12	2.48	0.44
1:F:130:LYS:HG3	1:F:131:VAL:N	2.33	0.44
1:A:163:PHE:HE2	1:A:199:LEU:HB3	1.83	0.44
1:D:130:LYS:HG3	1:D:131:VAL:N	2.33	0.44
1:E:154:VAL:O	1:E:158:LEU:CD2	2.65	0.44
1:C:154:VAL:O	1:C:158:LEU:CD2	2.65	0.44
1:A:178:GLY:O	1:A:179:GLU:HB3	2.17	0.44
1:G:178:GLY:O	1:G:179:GLU:CB	2.65	0.44
1:H:18:VAL:C	1:H:19:ILE:HG12	2.35	0.44
1:A:165:ALA:O	1:A:169:GLU:HB2	2.17	0.44
1:A:58:THR:HG22	1:A:59:LEU:N	2.32	0.44
1:E:163:PHE:CE2	1:E:199:LEU:HD22	2.53	0.44
1:D:60:TYR:CD1	1:D:60:TYR:N	2.85	0.44
1:A:154:VAL:O	1:A:158:LEU:CD2	2.66	0.44
1:E:192:LEU:O	1:E:195:ALA:N	2.31	0.44
1:F:154:VAL:O	1:F:155:VAL:C	2.56	0.44
1:E:178:GLY:O	1:E:179:GLU:HB3	2.17	0.44
1:G:105:ASP:CB	1:G:108:SER:OG	2.66	0.44
1:D:3:PHE:HA	1:D:48:THR:CG2	2.43	0.43
1:E:8:GLU:HG2	1:E:10:LEU:CD2	2.48	0.43
1:F:70:LEU:O	1:F:73:ALA:CB	2.63	0.43
1:F:95:ALA:C	1:F:97:LEU:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ALA:C	1:B:97:LEU:N	2.70	0.43
1:H:95:ALA:C	1:H:97:LEU:N	2.71	0.43
1:E:61:GLY:C	1:E:62:PHE:CG	2.91	0.43
1:F:14:LEU:CD1	1:F:14:LEU:H	2.10	0.43
1:A:192:LEU:C	1:A:194:ALA:H	2.21	0.43
1:B:195:ALA:O	1:B:198:LEU:N	2.51	0.43
1:F:195:ALA:O	1:F:198:LEU:N	2.51	0.43
1:G:97:LEU:HD12	1:G:97:LEU:HA	1.83	0.43
1:F:31:THR:HB	1:F:32:PRO:HD2	1.99	0.43
1:A:163:PHE:CE2	1:A:199:LEU:HD22	2.53	0.43
1:H:29:ASN:HD22	1:H:29:ASN:N	2.15	0.43
1:G:155:VAL:HG22	1:G:156:GLU:N	2.32	0.43
1:E:173:ASP:O	1:E:177:ASP:OD1	2.36	0.43
1:C:178:GLY:O	1:C:179:GLU:CB	2.65	0.43
1:E:103:ASP:O	1:E:105:ASP:N	2.51	0.43
1:H:62:PHE:CD1	1:H:62:PHE:N	2.86	0.43
1:G:64:ASP:OD1	1:G:64:ASP:C	2.56	0.43
1:C:8:GLU:CG	1:C:8:GLU:O	2.65	0.43
1:D:21:ALA:N	1:D:24:ILE:O	2.51	0.43
1:E:29:ASN:O	1:E:29:ASN:OD1	2.36	0.43
1:F:31:THR:HG22	1:F:86:MET:HE3	1.96	0.43
1:F:60:TYR:CD1	1:F:60:TYR:N	2.85	0.43
1:C:84:LEU:O	1:C:87:ALA:HB3	2.18	0.43
1:H:189:SER:C	1:H:191:ALA:H	2.22	0.43
1:H:195:ALA:O	1:H:198:LEU:N	2.51	0.43
1:C:31:THR:O	1:C:32:PRO:C	2.57	0.43
1:H:121:GLU:O	1:H:122:ARG:C	2.56	0.43
1:F:31:THR:CA	1:F:35:LEU:HD12	2.47	0.43
1:E:27:ARG:HG3	1:F:3:PHE:CE2	2.53	0.43
1:F:70:LEU:O	1:F:74:LEU:N	2.49	0.43
1:G:29:ASN:O	1:G:29:ASN:OD1	2.36	0.43
1:G:163:PHE:CE2	1:G:199:LEU:HD22	2.53	0.43
1:E:163:PHE:HE2	1:E:199:LEU:HB3	1.83	0.43
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.80	0.43
1:A:61:GLY:C	1:A:62:PHE:CG	2.92	0.43
1:E:155:VAL:HG22	1:E:156:GLU:N	2.32	0.43
1:A:14:LEU:O	1:A:35:LEU:HD22	2.18	0.43
1:C:31:THR:C	1:C:35:LEU:CD1	2.86	0.43
1:G:50:MET:HA	1:G:58:THR:O	2.17	0.43
1:G:120:ALA:O	1:G:121:GLU:C	2.56	0.43
1:E:165:ALA:O	1:E:169:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:O	1:C:169:GLU:HB2	2.18	0.43
1:B:70:LEU:O	1:B:74:LEU:N	2.49	0.43
1:H:3:PHE:HA	1:H:48:THR:CG2	2.44	0.43
1:F:110:THR:O	1:F:111:ARG:C	2.57	0.43
1:D:109:LEU:O	1:D:112:VAL:HG13	2.18	0.43
1:B:106:VAL:O	1:B:107:ALA:C	2.56	0.43
1:E:190:SER:O	1:E:194:ALA:CB	2.67	0.43
1:C:192:LEU:C	1:C:194:ALA:H	2.22	0.43
1:C:178:GLY:O	1:C:179:GLU:HB3	2.17	0.43
1:C:103:ASP:O	1:C:105:ASP:N	2.52	0.43
1:H:169:GLU:H	1:H:169:GLU:HG2	1.55	0.43
1:C:32:PRO:O	1:C:33:SER:C	2.57	0.43
1:F:28:VAL:HG12	1:F:28:VAL:O	2.17	0.43
1:D:34:ALA:C	1:D:36:ALA:N	2.70	0.43
1:A:113:PRO:HG3	1:B:163:PHE:CD1	2.53	0.43
1:F:106:VAL:O	1:F:107:ALA:C	2.57	0.43
1:E:99:GLN:O	1:E:100:ALA:C	2.55	0.43
1:F:175:VAL:O	1:F:176:LEU:C	2.55	0.43
1:H:123:ILE:H	1:H:123:ILE:HG12	1.62	0.43
1:E:31:THR:C	1:E:35:LEU:CD1	2.86	0.43
1:E:84:LEU:O	1:E:87:ALA:HB3	2.18	0.43
1:C:163:PHE:HE2	1:C:199:LEU:HB3	1.84	0.43
1:G:61:GLY:C	1:G:62:PHE:CG	2.91	0.43
1:C:97:LEU:HA	1:C:97:LEU:HD12	1.84	0.43
1:A:103:ASP:O	1:A:105:ASP:N	2.51	0.43
1:E:31:THR:O	1:E:32:PRO:C	2.56	0.43
1:D:71:PHE:HA	1:D:74:LEU:CD1	2.48	0.43
1:F:16:HIS:CD2	1:F:29:ASN:ND2	2.87	0.43
1:F:80:VAL:HG23	1:F:81:GLY:H	1.84	0.43
1:H:31:THR:HB	1:H:32:PRO:HD2	1.99	0.43
1:B:91:VAL:HG21	1:B:112:VAL:HG12	2.00	0.43
1:E:128:ALA:O	1:E:131:VAL:HB	2.19	0.43
1:H:193:ARG:CG	1:H:193:ARG:NH1	2.82	0.43
1:C:190:SER:O	1:C:194:ALA:CB	2.67	0.43
1:B:154:VAL:O	1:B:155:VAL:C	2.56	0.43
1:E:94:ALA:O	1:E:97:LEU:N	2.52	0.43
1:A:149:ALA:C	1:A:151:ARG:N	2.69	0.43
1:C:16:HIS:CA	1:C:29:ASN:HA	2.47	0.43
1:D:31:THR:CA	1:D:35:LEU:HD12	2.48	0.43
1:F:91:VAL:HG21	1:F:112:VAL:HG12	2.00	0.43
1:E:71:PHE:CE1	1:E:85:ALA:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:ASP:OD2	1:H:107:ALA:HB3	2.19	0.43
1:C:128:ALA:O	1:C:131:VAL:HB	2.19	0.43
1:B:60:TYR:N	1:B:60:TYR:CD1	2.86	0.43
1:A:152:GLY:C	1:A:155:VAL:HG13	2.39	0.43
1:B:62:PHE:N	1:B:62:PHE:CD1	2.87	0.43
1:G:8:GLU:HG2	1:G:10:LEU:CD2	2.49	0.43
1:A:29:ASN:O	1:A:29:ASN:OD1	2.36	0.43
1:G:112:VAL:HG13	1:G:113:PRO:CD	2.47	0.43
1:F:105:ASP:OD2	1:F:107:ALA:HB3	2.19	0.43
1:F:108:SER:OG	1:F:109:LEU:N	2.50	0.43
1:C:70:LEU:O	1:C:71:PHE:C	2.57	0.43
1:C:71:PHE:CE1	1:C:85:ALA:HB3	2.53	0.43
1:H:91:VAL:HG21	1:H:112:VAL:HG12	2.00	0.43
1:D:16:HIS:CD2	1:D:29:ASN:ND2	2.87	0.43
1:G:7:GLY:O	1:G:43:GLN:HA	2.19	0.43
1:B:121:GLU:O	1:B:122:ARG:C	2.56	0.43
1:B:21:ALA:N	1:B:24:ILE:O	2.52	0.42
1:F:17:ALA:HB2	1:F:35:LEU:CD2	2.49	0.42
1:F:70:LEU:O	1:F:71:PHE:C	2.58	0.42
1:A:70:LEU:O	1:A:71:PHE:C	2.57	0.42
1:A:80:VAL:CG1	1:A:80:VAL:O	2.66	0.42
1:G:113:PRO:HG3	1:H:163:PHE:CD1	2.54	0.42
1:C:201:LYS:O	1:C:202:THR:C	2.57	0.42
1:G:6:ARG:HG3	1:G:45:ARG:CB	2.40	0.42
1:D:46:LEU:HG	1:D:46:LEU:O	2.19	0.42
1:A:32:PRO:O	1:A:33:SER:C	2.57	0.42
1:C:27:ARG:HG3	1:D:3:PHE:CE2	2.55	0.42
1:A:27:ARG:HG3	1:B:3:PHE:CE2	2.54	0.42
1:B:34:ALA:O	1:B:36:ALA:N	2.52	0.42
1:G:71:PHE:CE1	1:G:85:ALA:HB3	2.54	0.42
1:H:52:VAL:O	1:H:53:ARG:NH1	2.49	0.42
1:E:130:LYS:HD3	1:E:130:LYS:HA	1.71	0.42
1:C:14:LEU:O	1:C:35:LEU:HD22	2.19	0.42
1:G:32:PRO:O	1:G:33:SER:C	2.57	0.42
1:H:70:LEU:O	1:H:73:ALA:CB	2.63	0.42
1:A:71:PHE:CE1	1:A:85:ALA:HB3	2.53	0.42
1:A:86:MET:O	1:A:89:LEU:N	2.52	0.42
1:G:84:LEU:HD21	1:G:114:GLY:O	2.19	0.42
1:G:201:LYS:O	1:G:202:THR:C	2.57	0.42
1:B:105:ASP:OD2	1:B:107:ALA:HB3	2.19	0.42
1:B:110:THR:O	1:B:111:ARG:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:PHE:CE2	1:C:199:LEU:HD22	2.54	0.42
1:H:109:LEU:HD23	1:H:109:LEU:HA	1.79	0.42
1:H:16:HIS:CD2	1:H:29:ASN:ND2	2.87	0.42
1:F:169:GLU:HG2	1:F:169:GLU:H	1.54	0.42
1:D:47:VAL:HB	1:D:62:PHE:O	2.19	0.42
1:B:46:LEU:HG	1:B:46:LEU:O	2.19	0.42
1:C:31:THR:HA	1:C:32:PRO:HD2	1.85	0.42
1:C:24:ILE:HG22	1:C:24:ILE:O	2.19	0.42
1:B:31:THR:CA	1:B:35:LEU:HD12	2.49	0.42
1:E:10:LEU:HB2	1:E:18:VAL:CG2	2.50	0.42
1:F:29:ASN:N	1:F:29:ASN:HD22	2.16	0.42
1:C:83:ARG:O	1:C:84:LEU:C	2.58	0.42
1:D:95:ALA:C	1:D:97:LEU:N	2.70	0.42
1:G:4:SER:C	1:G:5:VAL:HG23	2.35	0.42
1:H:46:LEU:O	1:H:46:LEU:HG	2.19	0.42
1:B:47:VAL:HB	1:B:62:PHE:O	2.19	0.42
1:E:120:ALA:O	1:E:121:GLU:C	2.58	0.42
1:E:50:MET:HA	1:E:58:THR:O	2.18	0.42
1:A:8:GLU:HG2	1:A:10:LEU:CD2	2.48	0.42
1:F:24:ILE:CG2	1:F:25:GLY:N	2.81	0.42
1:F:105:ASP:OD1	1:F:106:VAL:C	2.58	0.42
1:D:105:ASP:OD1	1:D:106:VAL:C	2.57	0.42
1:B:100:ALA:O	1:B:101:LEU:C	2.57	0.42
1:D:189:SER:C	1:D:191:ALA:H	2.22	0.42
1:A:173:ASP:O	1:A:177:ASP:OD1	2.36	0.42
1:H:195:ALA:O	1:H:198:LEU:HB3	2.19	0.42
1:H:21:ALA:N	1:H:24:ILE:O	2.52	0.42
1:C:120:ALA:O	1:C:121:GLU:C	2.57	0.42
1:B:36:ALA:O	1:B:38:LEU:N	2.51	0.42
1:A:84:LEU:HD21	1:A:114:GLY:O	2.20	0.42
1:G:109:LEU:C	1:G:111:ARG:N	2.73	0.42
1:A:201:LYS:O	1:A:202:THR:C	2.57	0.42
1:B:97:LEU:C	1:B:99:GLN:N	2.72	0.42
1:E:163:PHE:CE1	1:H:112:VAL:HA	2.42	0.42
1:B:189:SER:C	1:B:191:ALA:H	2.22	0.42
1:G:130:LYS:HA	1:G:130:LYS:HD3	1.70	0.42
1:D:46:LEU:CD1	1:D:46:LEU:C	2.83	0.42
1:H:20:GLU:HA	1:H:25:GLY:HA2	2.02	0.42
1:B:71:PHE:HA	1:B:74:LEU:CD1	2.50	0.42
1:H:17:ALA:HB2	1:H:35:LEU:CD2	2.50	0.42
1:H:81:GLY:C	1:H:83:ARG:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:O	1:B:112:VAL:O	2.37	0.42
1:B:16:HIS:CD2	1:B:29:ASN:ND2	2.88	0.42
1:G:192:LEU:C	1:G:194:ALA:H	2.22	0.42
1:F:195:ALA:O	1:F:198:LEU:HB3	2.19	0.42
1:H:46:LEU:CD1	1:H:46:LEU:C	2.82	0.42
1:F:47:VAL:HB	1:F:62:PHE:O	2.19	0.42
1:G:24:ILE:O	1:G:24:ILE:HG22	2.19	0.42
1:E:122:ARG:O	1:E:123:ILE:C	2.58	0.42
1:H:60:TYR:CD1	1:H:60:TYR:N	2.86	0.42
1:E:64:ASP:C	1:E:64:ASP:OD1	2.58	0.42
1:A:2:ILE:HG12	1:D:24:ILE:HG21	2.01	0.42
1:C:10:LEU:HB2	1:C:18:VAL:CG2	2.49	0.42
1:D:36:ALA:O	1:D:38:LEU:N	2.51	0.42
1:B:20:GLU:HA	1:B:25:GLY:HA2	2.02	0.42
1:B:32:PRO:O	1:B:33:SER:C	2.58	0.42
1:G:27:ARG:HG3	1:H:3:PHE:CE2	2.54	0.42
1:H:32:PRO:O	1:H:33:SER:C	2.58	0.42
1:H:71:PHE:HA	1:H:74:LEU:CD1	2.49	0.42
1:D:100:ALA:O	1:D:101:LEU:C	2.58	0.42
1:D:110:THR:O	1:D:112:VAL:O	2.38	0.42
1:A:173:ASP:HA	1:A:176:LEU:CD2	2.39	0.42
1:C:110:THR:HA	1:C:115:ILE:CG2	2.45	0.42
1:D:195:ALA:O	1:D:198:LEU:N	2.51	0.42
1:E:130:LYS:CD	1:E:134:VAL:HB	2.48	0.42
1:F:62:PHE:CD1	1:F:62:PHE:N	2.88	0.42
1:H:24:ILE:CG2	1:H:25:GLY:N	2.80	0.42
1:D:70:LEU:O	1:D:71:PHE:C	2.58	0.42
1:B:80:VAL:HG23	1:B:81:GLY:H	1.85	0.42
1:B:82:PRO:HA	1:B:85:ALA:HB3	2.02	0.42
1:A:122:ARG:O	1:A:123:ILE:C	2.57	0.42
1:E:30:ALA:HA	1:E:86:MET:HE2	2.01	0.42
1:D:97:LEU:C	1:D:99:GLN:N	2.72	0.42
1:E:162:GLY:O	1:E:163:PHE:C	2.58	0.42
1:E:201:LYS:O	1:E:202:THR:C	2.57	0.42
1:H:100:ALA:O	1:H:101:LEU:C	2.58	0.42
1:D:29:ASN:O	1:D:60:TYR:HA	2.20	0.42
1:B:29:ASN:N	1:B:29:ASN:HD22	2.17	0.42
1:G:152:GLY:C	1:G:155:VAL:HG13	2.40	0.42
1:E:14:LEU:O	1:E:35:LEU:HD22	2.20	0.42
1:E:2:ILE:HB	1:E:50:MET:HE2	2.02	0.42
1:D:34:ALA:O	1:D:36:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LEU:O	1:F:112:VAL:HG13	2.20	0.42
1:E:113:PRO:HG3	1:F:163:PHE:CD1	2.55	0.42
1:B:105:ASP:O	1:B:106:VAL:CB	2.68	0.42
1:H:109:LEU:O	1:H:112:VAL:HG13	2.19	0.42
1:B:14:LEU:HD12	1:B:14:LEU:N	2.14	0.42
1:C:192:LEU:O	1:C:196:LEU:N	2.51	0.42
1:B:123:ILE:H	1:B:123:ILE:HG12	1.64	0.42
1:G:10:LEU:HB2	1:G:18:VAL:CG2	2.50	0.42
1:G:14:LEU:O	1:G:35:LEU:HD22	2.20	0.42
1:D:28:VAL:O	1:D:28:VAL:HG12	2.19	0.42
1:B:28:VAL:HG12	1:B:28:VAL:O	2.20	0.42
1:H:17:ALA:HB2	1:H:35:LEU:HD23	2.02	0.41
1:H:80:VAL:HG23	1:H:81:GLY:H	1.85	0.41
1:H:106:VAL:O	1:H:107:ALA:C	2.57	0.41
1:B:154:VAL:HG11	1:B:172:THR:HG23	2.02	0.41
1:C:2:ILE:HB	1:C:50:MET:HE2	2.02	0.41
1:B:21:ALA:HB3	1:B:26:TYR:HE1	1.85	0.41
1:F:34:ALA:O	1:F:36:ALA:N	2.53	0.41
1:F:71:PHE:HA	1:F:74:LEU:CD1	2.50	0.41
1:F:81:GLY:C	1:F:83:ARG:N	2.73	0.41
1:F:83:ARG:H	1:F:83:ARG:HG2	1.59	0.41
1:G:87:ALA:O	1:G:88:THR:C	2.58	0.41
1:E:84:LEU:HD21	1:E:114:GLY:O	2.20	0.41
1:D:105:ASP:OD2	1:D:107:ALA:HB3	2.20	0.41
1:B:105:ASP:OD1	1:B:106:VAL:C	2.59	0.41
1:A:190:SER:O	1:A:194:ALA:CB	2.68	0.41
1:E:152:GLY:C	1:E:155:VAL:HG13	2.41	0.41
1:H:156:GLU:O	1:H:159:VAL:HB	2.20	0.41
1:D:195:ALA:O	1:D:198:LEU:HB3	2.19	0.41
1:C:64:ASP:C	1:C:64:ASP:OD1	2.58	0.41
1:C:18:VAL:HG12	1:C:27:ARG:HA	2.02	0.41
1:B:37:THR:O	1:B:38:LEU:HD13	2.20	0.41
1:B:3:PHE:HA	1:B:48:THR:CG2	2.44	0.41
1:B:70:LEU:O	1:B:71:PHE:C	2.58	0.41
1:F:32:PRO:O	1:F:33:SER:C	2.58	0.41
1:F:35:LEU:HA	1:F:38:LEU:CD2	2.47	0.41
1:G:162:GLY:O	1:G:163:PHE:C	2.58	0.41
1:A:128:ALA:O	1:A:131:VAL:HB	2.19	0.41
1:C:154:VAL:O	1:C:154:VAL:HG12	2.20	0.41
1:B:195:ALA:O	1:B:198:LEU:HB3	2.19	0.41
1:B:39:ASN:O	1:B:40:GLN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:ARG:O	1:G:123:ILE:C	2.57	0.41
1:D:91:VAL:HG21	1:D:112:VAL:HG12	2.01	0.41
1:C:162:GLY:O	1:C:163:PHE:C	2.58	0.41
1:H:105:ASP:OD1	1:H:106:VAL:C	2.58	0.41
1:E:192:LEU:C	1:E:194:ALA:H	2.22	0.41
1:D:20:GLU:HA	1:D:25:GLY:HA2	2.02	0.41
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.50	0.41
1:F:17:ALA:HB2	1:F:35:LEU:HD23	2.02	0.41
1:H:70:LEU:O	1:H:71:PHE:C	2.57	0.41
1:A:112:VAL:HG13	1:A:113:PRO:CD	2.47	0.41
1:E:80:VAL:CG1	1:E:80:VAL:O	2.66	0.41
1:E:83:ARG:O	1:E:84:LEU:C	2.58	0.41
1:D:106:VAL:O	1:D:107:ALA:C	2.57	0.41
1:G:154:VAL:HG12	1:G:154:VAL:O	2.20	0.41
1:G:103:ASP:O	1:G:105:ASP:N	2.53	0.41
1:H:39:ASN:O	1:H:40:GLN:C	2.59	0.41
1:A:64:ASP:C	1:A:64:ASP:OD1	2.58	0.41
1:D:17:ALA:HB2	1:D:35:LEU:CD2	2.51	0.41
1:D:3:PHE:CA	1:D:48:THR:HG22	2.45	0.41
1:F:21:ALA:N	1:F:24:ILE:O	2.53	0.41
1:C:131:VAL:O	1:C:131:VAL:HG12	2.21	0.41
1:C:157:ALA:O	1:C:158:LEU:C	2.59	0.41
1:G:190:SER:O	1:G:194:ALA:CB	2.68	0.41
1:H:156:GLU:O	1:H:159:VAL:N	2.54	0.41
1:A:83:ARG:O	1:A:84:LEU:C	2.58	0.41
1:C:30:ALA:HA	1:C:86:MET:HE2	2.02	0.41
1:H:103:ASP:O	1:H:104:SER:C	2.59	0.41
1:C:154:VAL:HG13	1:C:192:LEU:HD22	2.02	0.41
1:C:152:GLY:C	1:C:155:VAL:HG13	2.41	0.41
1:A:97:LEU:HD12	1:A:97:LEU:HA	1.84	0.41
1:F:39:ASN:O	1:F:40:GLN:C	2.59	0.41
1:G:31:THR:HA	1:G:32:PRO:HD2	1.84	0.41
1:H:28:VAL:HG12	1:H:28:VAL:O	2.20	0.41
1:A:18:VAL:HG12	1:A:27:ARG:HA	2.02	0.41
1:F:15:ASP:CG	1:F:16:HIS:H	2.24	0.41
1:B:16:HIS:CE1	1:B:27:ARG:CD	3.04	0.41
1:B:29:ASN:O	1:B:60:TYR:HA	2.20	0.41
1:F:89:LEU:HD23	1:F:89:LEU:HA	1.86	0.41
1:D:32:PRO:O	1:D:33:SER:C	2.58	0.41
1:D:37:THR:O	1:D:38:LEU:HD13	2.21	0.41
1:F:16:HIS:CE1	1:F:27:ARG:CD	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LEU:HA	1:F:38:LEU:HD12	1.98	0.41
1:F:29:ASN:O	1:F:60:TYR:HA	2.20	0.41
1:A:123:ILE:O	1:A:126:GLU:HB2	2.21	0.41
1:A:109:LEU:C	1:A:111:ARG:N	2.74	0.41
1:G:83:ARG:O	1:G:84:LEU:C	2.58	0.41
1:F:100:ALA:O	1:F:101:LEU:C	2.58	0.41
1:F:109:LEU:HD12	1:F:120:ALA:HB1	2.03	0.41
1:D:103:ASP:O	1:D:104:SER:C	2.59	0.41
1:B:95:ALA:O	1:B:97:LEU:C	2.60	0.41
1:H:110:THR:O	1:H:111:ARG:C	2.57	0.41
1:E:131:VAL:HG12	1:E:131:VAL:O	2.21	0.41
1:C:129:ASP:C	1:C:131:VAL:N	2.75	0.41
1:D:16:HIS:CE1	1:D:27:ARG:CD	3.04	0.41
1:H:16:HIS:CE1	1:H:27:ARG:CD	3.03	0.41
1:F:202:THR:CG2	1:F:203:ARG:HH21	2.34	0.41
1:D:156:GLU:O	1:D:159:VAL:N	2.54	0.41
1:B:156:GLU:O	1:B:159:VAL:HB	2.21	0.41
1:D:62:PHE:N	1:D:62:PHE:CD1	2.88	0.41
1:C:7:GLY:O	1:C:43:GLN:HA	2.20	0.41
1:A:7:GLY:O	1:A:43:GLN:HA	2.21	0.41
1:H:89:LEU:HD23	1:H:89:LEU:HA	1.86	0.41
1:C:122:ARG:O	1:C:123:ILE:C	2.58	0.41
1:F:21:ALA:HB3	1:F:26:TYR:HE1	1.86	0.41
1:F:110:THR:O	1:F:112:VAL:O	2.38	0.41
1:C:88:THR:O	1:C:91:VAL:N	2.54	0.41
1:E:154:VAL:HG13	1:E:192:LEU:HD22	2.02	0.41
1:F:156:GLU:O	1:F:159:VAL:N	2.54	0.41
1:B:169:GLU:O	1:B:171:ALA:N	2.54	0.41
1:A:130:LYS:HA	1:A:130:LYS:HD3	1.69	0.41
1:A:24:ILE:HG22	1:A:24:ILE:O	2.20	0.40
1:A:16:HIS:CA	1:A:29:ASN:HA	2.48	0.40
1:F:20:GLU:HA	1:F:25:GLY:HA2	2.02	0.40
1:A:30:ALA:HA	1:A:86:MET:HE2	2.03	0.40
1:E:109:LEU:C	1:E:111:ARG:N	2.74	0.40
1:D:105:ASP:O	1:D:106:VAL:CB	2.69	0.40
1:B:106:VAL:O	1:B:107:ALA:O	2.39	0.40
1:H:95:ALA:O	1:H:97:LEU:C	2.59	0.40
1:G:128:ALA:O	1:G:131:VAL:HB	2.19	0.40
1:E:154:VAL:O	1:E:154:VAL:HG12	2.20	0.40
1:E:20:GLU:O	1:E:20:GLU:CG	2.69	0.40
1:H:195:ALA:O	1:H:199:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:VAL:HG11	1:F:172:THR:HG23	2.02	0.40
1:E:7:GLY:O	1:E:43:GLN:HA	2.21	0.40
1:D:38:LEU:HD12	1:D:38:LEU:HA	1.97	0.40
1:B:17:ALA:HB2	1:B:35:LEU:CD2	2.50	0.40
1:C:87:ALA:O	1:C:88:THR:C	2.59	0.40
1:D:106:VAL:O	1:D:107:ALA:O	2.39	0.40
1:A:154:VAL:O	1:A:154:VAL:HG12	2.20	0.40
1:G:173:ASP:HA	1:G:176:LEU:CD2	2.39	0.40
1:C:113:PRO:O	1:C:115:ILE:N	2.54	0.40
1:D:81:GLY:C	1:D:83:ARG:N	2.73	0.40
1:D:83:ARG:HG3	1:D:84:LEU:CD1	2.52	0.40
1:B:81:GLY:C	1:B:83:ARG:N	2.73	0.40
1:G:109:LEU:O	1:G:112:VAL:N	2.54	0.40
1:F:105:ASP:O	1:F:106:VAL:CB	2.70	0.40
1:F:95:ALA:O	1:F:97:LEU:C	2.59	0.40
1:C:70:LEU:O	1:C:74:LEU:N	2.41	0.40
1:E:129:ASP:C	1:E:131:VAL:N	2.75	0.40
1:A:131:VAL:HG12	1:A:131:VAL:O	2.22	0.40
1:A:153:SER:OG	1:A:188:THR:HG21	2.21	0.40
1:C:112:VAL:HG13	1:C:113:PRO:CD	2.47	0.40
1:F:46:LEU:O	1:F:46:LEU:HG	2.21	0.40
1:G:164:ALA:O	1:G:166:LYS:N	2.55	0.40
1:D:35:LEU:HA	1:D:38:LEU:CD2	2.47	0.40
1:E:24:ILE:O	1:E:24:ILE:HG22	2.21	0.40
1:E:16:HIS:CA	1:E:29:ASN:HA	2.49	0.40
1:H:34:ALA:O	1:H:36:ALA:N	2.54	0.40
1:A:113:PRO:O	1:A:115:ILE:N	2.55	0.40
1:G:77:VAL:O	1:G:80:VAL:CG1	2.67	0.40
1:A:162:GLY:O	1:A:163:PHE:C	2.58	0.40
1:D:125:LEU:HD23	1:D:126:GLU:HB2	2.03	0.40
1:H:110:THR:O	1:H:112:VAL:O	2.38	0.40
1:G:131:VAL:O	1:G:131:VAL:HG12	2.21	0.40
1:D:165:ALA:O	1:D:167:GLN:N	2.55	0.40
1:D:39:ASN:O	1:D:40:GLN:C	2.60	0.40
1:D:82:PRO:HA	1:D:85:ALA:HB3	2.04	0.40
1:E:18:VAL:HG12	1:E:27:ARG:HA	2.02	0.40
1:F:82:PRO:HA	1:F:85:ALA:HB3	2.02	0.40
1:G:123:ILE:O	1:G:126:GLU:HB2	2.22	0.40
1:G:70:LEU:O	1:G:71:PHE:C	2.59	0.40
1:F:97:LEU:C	1:F:99:GLN:N	2.71	0.40
1:C:80:VAL:CG1	1:C:80:VAL:O	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:LEU:C	1:H:99:GLN:N	2.72	0.40
1:F:192:LEU:C	1:F:194:ALA:H	2.25	0.40
1:E:153:SER:OG	1:E:188:THR:HG21	2.22	0.40
1:G:154:VAL:HG23	1:G:188:THR:HG22	2.03	0.40
1:G:154:VAL:HG13	1:G:192:LEU:HD22	2.03	0.40
1:C:109:LEU:C	1:C:111:ARG:N	2.74	0.40
1:D:154:VAL:HG11	1:D:172:THR:HG23	2.02	0.40
1:D:202:THR:CG2	1:D:203:ARG:HH21	2.34	0.40
1:E:68:ARG:O	1:E:69:ASP:C	2.60	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	177/203 (87%)	96 (54%)	58 (33%)	23 (13%)	0	1
1	B	177/203 (87%)	78 (44%)	58 (33%)	41 (23%)	0	0
1	C	177/203 (87%)	95 (54%)	59 (33%)	23 (13%)	0	1
1	D	177/203 (87%)	78 (44%)	58 (33%)	41 (23%)	0	0
1	E	177/203 (87%)	91 (51%)	62 (35%)	24 (14%)	0	1
1	F	177/203 (87%)	78 (44%)	58 (33%)	41 (23%)	0	0
1	G	177/203 (87%)	94 (53%)	60 (34%)	23 (13%)	0	1
1	H	177/203 (87%)	78 (44%)	58 (33%)	41 (23%)	0	0
All	All	1416/1624 (87%)	688 (49%)	471 (33%)	257 (18%)	0	0

All (257) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL

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Mol	Chain	Res	Type
1	A	105	ASP
1	A	110	THR
1	A	133	PRO
1	A	176	LEU
1	B	80	VAL
1	B	85	ALA
1	B	91	VAL
1	B	93	ASP
1	B	96	ALA
1	B	99	GLN
1	B	109	LEU
1	B	110	THR
1	B	117	ARG
1	B	129	ASP
1	B	131	VAL
1	B	171	ALA
1	B	188	THR
1	B	191	ALA
1	B	192	LEU
1	B	199	LEU
1	B	201	LYS
1	C	5	VAL
1	C	105	ASP
1	C	110	THR
1	C	133	PRO
1	C	176	LEU
1	D	80	VAL
1	D	85	ALA
1	D	91	VAL
1	D	93	ASP
1	D	96	ALA
1	D	99	GLN
1	D	109	LEU
1	D	110	THR
1	D	117	ARG
1	D	129	ASP
1	D	131	VAL
1	D	171	ALA
1	D	188	THR
1	D	191	ALA
1	D	192	LEU
1	D	199	LEU

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Mol	Chain	Res	Type
1	D	201	LYS
1	E	5	VAL
1	E	105	ASP
1	E	110	THR
1	E	133	PRO
1	E	176	LEU
1	F	80	VAL
1	F	85	ALA
1	F	91	VAL
1	F	93	ASP
1	F	96	ALA
1	F	99	GLN
1	F	109	LEU
1	F	110	THR
1	F	117	ARG
1	F	129	ASP
1	F	131	VAL
1	F	171	ALA
1	F	188	THR
1	F	191	ALA
1	F	192	LEU
1	F	199	LEU
1	F	201	LYS
1	G	5	VAL
1	G	105	ASP
1	G	110	THR
1	G	133	PRO
1	G	176	LEU
1	H	80	VAL
1	H	85	ALA
1	H	91	VAL
1	H	93	ASP
1	H	96	ALA
1	H	99	GLN
1	H	109	LEU
1	H	110	THR
1	H	117	ARG
1	H	129	ASP
1	H	131	VAL
1	H	171	ALA
1	H	188	THR
1	H	191	ALA

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Mol	Chain	Res	Type
1	H	192	LEU
1	H	199	LEU
1	H	201	LYS
1	A	65	ALA
1	A	66	GLU
1	A	102	ALA
1	A	111	ARG
1	A	171	ALA
1	B	13	ALA
1	B	79	GLY
1	B	94	ALA
1	B	95	ALA
1	B	100	ALA
1	B	102	ALA
1	B	107	ALA
1	B	114	GLY
1	B	130	LYS
1	B	154	VAL
1	B	167	GLN
1	C	65	ALA
1	C	66	GLU
1	C	102	ALA
1	C	111	ARG
1	C	171	ALA
1	D	13	ALA
1	D	79	GLY
1	D	94	ALA
1	D	95	ALA
1	D	100	ALA
1	D	107	ALA
1	D	114	GLY
1	D	130	LYS
1	D	154	VAL
1	D	167	GLN
1	E	65	ALA
1	E	66	GLU
1	E	102	ALA
1	E	111	ARG
1	E	171	ALA
1	F	13	ALA
1	F	79	GLY
1	F	94	ALA

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Mol	Chain	Res	Type
1	F	95	ALA
1	F	100	ALA
1	F	102	ALA
1	F	107	ALA
1	F	114	GLY
1	F	130	LYS
1	F	167	GLN
1	G	65	ALA
1	G	66	GLU
1	G	102	ALA
1	G	111	ARG
1	G	171	ALA
1	H	13	ALA
1	H	79	GLY
1	H	83	ARG
1	H	94	ALA
1	H	95	ALA
1	H	100	ALA
1	H	102	ALA
1	H	107	ALA
1	H	114	GLY
1	H	130	LYS
1	H	154	VAL
1	H	167	GLN
1	H	174	GLN
1	A	54	GLU
1	A	104	SER
1	A	174	GLN
1	B	22	ALA
1	B	67	ASN
1	B	83	ARG
1	B	132	GLY
1	B	174	GLN
1	C	54	GLU
1	C	104	SER
1	C	174	GLN
1	D	22	ALA
1	D	67	ASN
1	D	83	ARG
1	D	84	LEU
1	D	102	ALA
1	D	132	GLY

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Mol	Chain	Res	Type
1	D	174	GLN
1	E	54	GLU
1	E	104	SER
1	E	174	GLN
1	F	22	ALA
1	F	67	ASN
1	F	83	ARG
1	F	132	GLY
1	F	154	VAL
1	F	174	GLN
1	G	54	GLU
1	G	104	SER
1	G	174	GLN
1	H	22	ALA
1	H	67	ASN
1	H	84	LEU
1	H	132	GLY
1	A	130	LYS
1	A	152	GLY
1	A	165	ALA
1	B	73	ALA
1	B	84	LEU
1	B	97	LEU
1	C	130	LYS
1	C	152	GLY
1	C	165	ALA
1	D	73	ALA
1	D	97	LEU
1	E	130	LYS
1	E	131	VAL
1	E	152	GLY
1	E	165	ALA
1	F	73	ALA
1	F	84	LEU
1	F	97	LEU
1	G	130	LYS
1	G	131	VAL
1	G	152	GLY
1	G	165	ALA
1	H	73	ALA
1	H	97	LEU
1	A	85	ALA

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Mol	Chain	Res	Type
1	A	87	ALA
1	A	97	LEU
1	A	131	VAL
1	B	40	GLN
1	B	44	ALA
1	B	98	ARG
1	B	178	GLY
1	C	85	ALA
1	C	87	ALA
1	C	97	LEU
1	C	131	VAL
1	D	40	GLN
1	D	44	ALA
1	D	178	GLY
1	E	85	ALA
1	E	97	LEU
1	F	40	GLN
1	F	44	ALA
1	F	98	ARG
1	F	178	GLY
1	G	85	ALA
1	G	87	ALA
1	G	97	LEU
1	H	40	GLN
1	H	44	ALA
1	H	98	ARG
1	H	178	GLY
1	B	155	VAL
1	D	98	ARG
1	D	155	VAL
1	E	16	HIS
1	E	87	ALA
1	F	155	VAL
1	H	155	VAL
1	A	154	VAL
1	C	154	VAL
1	E	154	VAL
1	G	154	VAL
1	A	32	PRO
1	C	32	PRO
1	E	32	PRO
1	G	32	PRO

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Mol	Chain	Res	Type
1	A	115	ILE
1	E	115	ILE
1	G	115	ILE
1	C	115	ILE

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	129/145 (89%)	82 (64%)	47 (36%)	0	1
1	B	131/145 (90%)	79 (60%)	52 (40%)	0	0
1	C	129/145 (89%)	82 (64%)	47 (36%)	0	1
1	D	131/145 (90%)	78 (60%)	53 (40%)	0	0
1	E	129/145 (89%)	80 (62%)	49 (38%)	0	1
1	F	131/145 (90%)	78 (60%)	53 (40%)	0	0
1	G	129/145 (89%)	81 (63%)	48 (37%)	0	1
1	H	131/145 (90%)	77 (59%)	54 (41%)	0	0
All	All	1040/1160 (90%)	637 (61%)	403 (39%)	0	0

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	8	GLU
1	A	14	LEU
1	A	16	HIS
1	A	20	GLU
1	A	24	ILE
1	A	27	ARG
1	A	33	SER
1	A	42	SER
1	A	45	ARG
1	A	50	MET

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Mol	Chain	Res	Type
1	A	53	ARG
1	A	63	SER
1	A	70	LEU
1	A	72	LEU
1	A	76	SER
1	A	78	SER
1	A	84	LEU
1	A	98	ARG
1	A	101	LEU
1	A	106	VAL
1	A	108	SER
1	A	115	ILE
1	A	118	ARG
1	A	121	GLU
1	A	126	GLU
1	A	130	LYS
1	A	151	ARG
1	A	155	VAL
1	A	159	VAL
1	A	161	LEU
1	A	166	LYS
1	A	167	GLN
1	A	169	GLU
1	A	172	THR
1	A	173	ASP
1	A	174	GLN
1	A	175	VAL
1	A	176	LEU
1	A	177	ASP
1	A	179	GLU
1	A	188	THR
1	A	190	SER
1	A	192	LEU
1	A	193	ARG
1	A	201	LYS
1	A	203	ARG
1	B	2	ILE
1	B	4	SER
1	B	6	ARG
1	B	11	GLU
1	B	14	LEU
1	B	15	ASP

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Mol	Chain	Res	Type
1	B	19	ILE
1	B	31	THR
1	B	38	LEU
1	B	43	GLN
1	B	46	LEU
1	B	48	THR
1	B	52	VAL
1	B	56	SER
1	B	57	MET
1	B	58	THR
1	B	62	PHE
1	B	68	ARG
1	B	70	LEU
1	B	76	SER
1	B	78	SER
1	B	80	VAL
1	B	83	ARG
1	B	84	LEU
1	B	86	MET
1	B	88	THR
1	B	101	LEU
1	B	104	SER
1	B	105	ASP
1	B	110	THR
1	B	112	VAL
1	B	115	ILE
1	B	118	ARG
1	B	121	GLU
1	B	124	VAL
1	B	125	LEU
1	B	126	GLU
1	B	129	ASP
1	B	131	VAL
1	B	148	ASN
1	B	151	ARG
1	B	153	SER
1	B	155	VAL
1	B	156	GLU
1	B	158	LEU
1	B	161	LEU
1	B	166	LYS
1	B	167	GLN

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Mol	Chain	Res	Type
1	B	189	SER
1	B	192	LEU
1	B	193	ARG
1	B	203	ARG
1	C	4	SER
1	C	8	GLU
1	C	14	LEU
1	C	16	HIS
1	C	20	GLU
1	C	24	ILE
1	C	27	ARG
1	C	33	SER
1	C	42	SER
1	C	45	ARG
1	C	50	MET
1	C	53	ARG
1	C	63	SER
1	C	70	LEU
1	C	72	LEU
1	C	76	SER
1	C	78	SER
1	C	84	LEU
1	C	98	ARG
1	C	101	LEU
1	C	106	VAL
1	C	108	SER
1	C	115	ILE
1	C	118	ARG
1	C	121	GLU
1	C	126	GLU
1	C	130	LYS
1	C	151	ARG
1	C	155	VAL
1	C	159	VAL
1	C	161	LEU
1	C	166	LYS
1	C	167	GLN
1	C	169	GLU
1	C	172	THR
1	C	173	ASP
1	C	174	GLN
1	C	175	VAL

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Mol	Chain	Res	Type
1	C	176	LEU
1	C	177	ASP
1	C	179	GLU
1	C	188	THR
1	C	190	SER
1	C	192	LEU
1	C	193	ARG
1	C	201	LYS
1	C	203	ARG
1	D	2	ILE
1	D	4	SER
1	D	6	ARG
1	D	11	GLU
1	D	14	LEU
1	D	15	ASP
1	D	19	ILE
1	D	31	THR
1	D	38	LEU
1	D	43	GLN
1	D	46	LEU
1	D	48	THR
1	D	52	VAL
1	D	56	SER
1	D	57	MET
1	D	58	THR
1	D	62	PHE
1	D	68	ARG
1	D	70	LEU
1	D	76	SER
1	D	78	SER
1	D	80	VAL
1	D	83	ARG
1	D	84	LEU
1	D	86	MET
1	D	88	THR
1	D	101	LEU
1	D	103	ASP
1	D	104	SER
1	D	105	ASP
1	D	110	THR
1	D	112	VAL
1	D	115	ILE

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Mol	Chain	Res	Type
1	D	118	ARG
1	D	121	GLU
1	D	124	VAL
1	D	125	LEU
1	D	126	GLU
1	D	129	ASP
1	D	131	VAL
1	D	148	ASN
1	D	151	ARG
1	D	153	SER
1	D	155	VAL
1	D	156	GLU
1	D	158	LEU
1	D	161	LEU
1	D	166	LYS
1	D	167	GLN
1	D	189	SER
1	D	192	LEU
1	D	193	ARG
1	D	203	ARG
1	E	4	SER
1	E	8	GLU
1	E	14	LEU
1	E	16	HIS
1	E	20	GLU
1	E	24	ILE
1	E	27	ARG
1	E	33	SER
1	E	42	SER
1	E	45	ARG
1	E	50	MET
1	E	53	ARG
1	E	63	SER
1	E	70	LEU
1	E	72	LEU
1	E	74	LEU
1	E	76	SER
1	E	78	SER
1	E	84	LEU
1	E	98	ARG
1	E	101	LEU
1	E	106	VAL

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Mol	Chain	Res	Type
1	E	108	SER
1	E	115	ILE
1	E	118	ARG
1	E	121	GLU
1	E	123	ILE
1	E	126	GLU
1	E	130	LYS
1	E	151	ARG
1	E	155	VAL
1	E	159	VAL
1	E	161	LEU
1	E	166	LYS
1	E	167	GLN
1	E	169	GLU
1	E	172	THR
1	E	173	ASP
1	E	174	GLN
1	E	175	VAL
1	E	176	LEU
1	E	177	ASP
1	E	179	GLU
1	E	188	THR
1	E	190	SER
1	E	192	LEU
1	E	193	ARG
1	E	201	LYS
1	E	203	ARG
1	F	2	ILE
1	F	4	SER
1	F	6	ARG
1	F	11	GLU
1	F	14	LEU
1	F	15	ASP
1	F	19	ILE
1	F	31	THR
1	F	38	LEU
1	F	43	GLN
1	F	46	LEU
1	F	48	THR
1	F	52	VAL
1	F	56	SER
1	F	57	MET

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Mol	Chain	Res	Type
1	F	58	THR
1	F	62	PHE
1	F	68	ARG
1	F	70	LEU
1	F	76	SER
1	F	78	SER
1	F	80	VAL
1	F	83	ARG
1	F	84	LEU
1	F	86	MET
1	F	88	THR
1	F	101	LEU
1	F	103	ASP
1	F	104	SER
1	F	105	ASP
1	F	110	THR
1	F	112	VAL
1	F	115	ILE
1	F	118	ARG
1	F	121	GLU
1	F	124	VAL
1	F	125	LEU
1	F	126	GLU
1	F	129	ASP
1	F	131	VAL
1	F	148	ASN
1	F	151	ARG
1	F	153	SER
1	F	155	VAL
1	F	156	GLU
1	F	158	LEU
1	F	161	LEU
1	F	166	LYS
1	F	167	GLN
1	F	189	SER
1	F	192	LEU
1	F	193	ARG
1	F	203	ARG
1	G	4	SER
1	G	8	GLU
1	G	14	LEU
1	G	16	HIS

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Mol	Chain	Res	Type
1	G	20	GLU
1	G	24	ILE
1	G	27	ARG
1	G	33	SER
1	G	42	SER
1	G	45	ARG
1	G	50	MET
1	G	53	ARG
1	G	63	SER
1	G	70	LEU
1	G	72	LEU
1	G	76	SER
1	G	78	SER
1	G	84	LEU
1	G	98	ARG
1	G	101	LEU
1	G	106	VAL
1	G	108	SER
1	G	115	ILE
1	G	118	ARG
1	G	121	GLU
1	G	123	ILE
1	G	126	GLU
1	G	130	LYS
1	G	151	ARG
1	G	155	VAL
1	G	159	VAL
1	G	161	LEU
1	G	166	LYS
1	G	167	GLN
1	G	169	GLU
1	G	172	THR
1	G	173	ASP
1	G	174	GLN
1	G	175	VAL
1	G	176	LEU
1	G	177	ASP
1	G	179	GLU
1	G	188	THR
1	G	190	SER
1	G	192	LEU
1	G	193	ARG

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Mol	Chain	Res	Type
1	G	201	LYS
1	G	203	ARG
1	H	2	ILE
1	H	4	SER
1	H	6	ARG
1	H	11	GLU
1	H	14	LEU
1	H	15	ASP
1	H	19	ILE
1	H	31	THR
1	H	38	LEU
1	H	43	GLN
1	H	46	LEU
1	H	48	THR
1	H	52	VAL
1	H	56	SER
1	H	57	MET
1	H	58	THR
1	H	62	PHE
1	H	68	ARG
1	H	70	LEU
1	H	76	SER
1	H	78	SER
1	H	80	VAL
1	H	83	ARG
1	H	84	LEU
1	H	86	MET
1	H	88	THR
1	H	101	LEU
1	H	103	ASP
1	H	104	SER
1	H	105	ASP
1	H	110	THR
1	H	112	VAL
1	H	115	ILE
1	H	118	ARG
1	H	121	GLU
1	H	124	VAL
1	H	125	LEU
1	H	126	GLU
1	H	129	ASP
1	H	131	VAL

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Mol	Chain	Res	Type
1	H	148	ASN
1	H	151	ARG
1	H	153	SER
1	H	155	VAL
1	H	156	GLU
1	H	158	LEU
1	H	161	LEU
1	H	166	LYS
1	H	167	GLN
1	H	169	GLU
1	H	189	SER
1	H	192	LEU
1	H	193	ARG
1	H	203	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	92	HIS
1	A	148	ASN
1	B	16	HIS
1	B	29	ASN
1	B	43	GLN
1	B	148	ASN
1	B	167	GLN
1	C	40	GLN
1	C	92	HIS
1	C	148	ASN
1	D	16	HIS
1	D	29	ASN
1	D	43	GLN
1	D	148	ASN
1	D	167	GLN
1	E	40	GLN
1	E	92	HIS
1	E	148	ASN
1	F	16	HIS
1	F	29	ASN
1	F	43	GLN
1	F	148	ASN
1	F	167	GLN

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Mol	Chain	Res	Type
1	G	40	GLN
1	G	92	HIS
1	G	148	ASN
1	H	16	HIS
1	H	29	ASN
1	H	43	GLN
1	H	148	ASN
1	H	167	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	183/203 (90%)	-0.00	8 (4%) 38 16	12, 36, 100, 100	0
1	B	183/203 (90%)	-0.30	1 (0%) 91 76	13, 40, 81, 100	0
1	C	183/203 (90%)	-0.07	8 (4%) 38 16	13, 35, 100, 100	0
1	D	183/203 (90%)	-0.32	0 100 100	13, 40, 83, 100	0
1	E	183/203 (90%)	-0.02	9 (4%) 33 13	9, 35, 100, 100	0
1	F	183/203 (90%)	-0.30	1 (0%) 91 76	12, 39, 80, 100	0
1	G	183/203 (90%)	-0.08	4 (2%) 65 35	13, 37, 99, 100	0
1	H	183/203 (90%)	-0.31	1 (0%) 91 76	14, 39, 80, 100	0
All	All	1464/1624 (90%)	-0.18	32 (2%) 65 35	9, 39, 96, 100	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	149	ALA	4.9
1	G	196	LEU	4.4
1	A	161	LEU	4.1
1	A	149	ALA	4.0
1	A	196	LEU	3.9
1	C	196	LEU	3.9
1	G	153	SER	3.7
1	A	176	LEU	3.5
1	C	149	ALA	3.5
1	E	196	LEU	3.5
1	C	176	LEU	3.5
1	A	153	SER	3.4
1	E	149	ALA	3.4
1	C	197	SER	3.2
1	B	203	ARG	3.0
1	E	176	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	161	LEU	2.7
1	H	203	ARG	2.7
1	E	197	SER	2.6
1	E	161	LEU	2.6
1	E	177	ASP	2.5
1	A	177	ASP	2.4
1	C	202	THR	2.3
1	E	163	PHE	2.3
1	E	153	SER	2.2
1	A	197	SER	2.2
1	C	153	SER	2.2
1	E	170	GLU	2.1
1	C	177	ASP	2.1
1	A	167	GLN	2.1
1	F	203	ARG	2.1
1	C	194	ALA	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.