



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:07 PM GMT

PDB ID : 3SR2  
Title : Crystal Structure of Human XLF-XRCC4 Complex  
Authors : Hammel, M.; Classen, S.; Tainer, J.A.  
Deposited on : 2011-07-06  
Resolution : 3.97 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](mailto: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.

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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

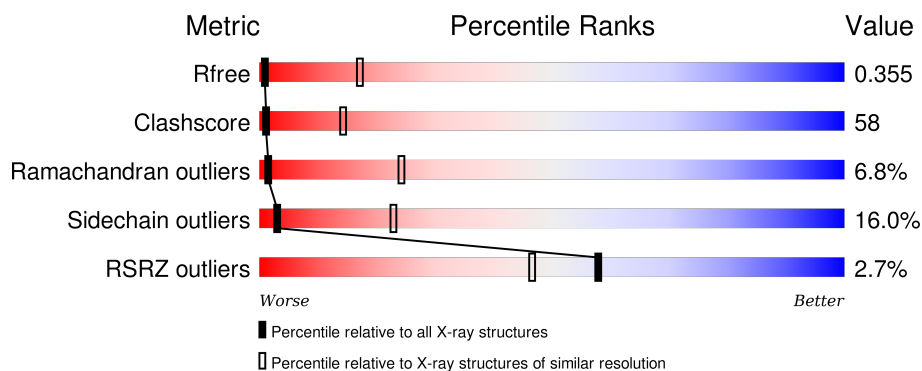
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.97 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	1009 (4.40-3.56)
Clashscore	102246	1033 (4.36-3.60)
Ramachandran outliers	100387	1012 (4.38-3.58)
Sidechain outliers	100360	1002 (4.38-3.58)
RSRZ outliers	91569	1012 (4.40-3.56)

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  $\geq 3$ , 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	145	<div> <div>20%</div> <div>56%</div> <div>19%</div> <div>• •</div> </div>
1	B	145	<div> <div>6%</div> <div>26%</div> <div>59%</div> <div>9%</div> <div>• •</div> </div>
1	E	145	<div> <div>2%</div> <div>45%</div> <div>41%</div> <div>9%</div> <div>• •</div> </div>
1	F	145	<div> <div>7%</div> <div>38%</div> <div>48%</div> <div>10%</div> <div>• •</div> </div>
2	C	229	<div> <div>27%</div> <div>57%</div> <div>11%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	229	 33% 51% 10% • 5%
2	G	229	 29% 52% 13% • 5%
2	H	229	 21% 51% 20% 5% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11363 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 DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1103	701	179	217	6			
1	B	140	Total	C	N	O	S	0	0	0
			1112	707	181	218	6			
1	E	140	Total	C	N	O	S	0	0	0
			1112	707	181	218	6			
1	F	140	Total	C	N	O	S	0	0	0
			1112	707	181	218	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q13426
A	-3	PRO	-	EXPRESSION TAG	UNP Q13426
A	-2	LEU	-	EXPRESSION TAG	UNP Q13426
A	-1	GLY	-	EXPRESSION TAG	UNP Q13426
A	0	SER	-	EXPRESSION TAG	UNP Q13426
B	-4	GLY	-	EXPRESSION TAG	UNP Q13426
B	-3	PRO	-	EXPRESSION TAG	UNP Q13426
B	-2	LEU	-	EXPRESSION TAG	UNP Q13426
B	-1	GLY	-	EXPRESSION TAG	UNP Q13426
B	0	SER	-	EXPRESSION TAG	UNP Q13426
E	-4	GLY	-	EXPRESSION TAG	UNP Q13426
E	-3	PRO	-	EXPRESSION TAG	UNP Q13426
E	-2	LEU	-	EXPRESSION TAG	UNP Q13426
E	-1	GLY	-	EXPRESSION TAG	UNP Q13426
E	0	SER	-	EXPRESSION TAG	UNP Q13426
F	-4	GLY	-	EXPRESSION TAG	UNP Q13426
F	-3	PRO	-	EXPRESSION TAG	UNP Q13426
F	-2	LEU	-	EXPRESSION TAG	UNP Q13426
F	-1	GLY	-	EXPRESSION TAG	UNP Q13426
F	0	SER	-	EXPRESSION TAG	UNP Q13426

- Molecule 2 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	218	Total	C	N	O	S	0	0	0
			1736	1112	290	319	15			
2	D	218	Total	C	N	O	S	0	0	0
			1720	1100	286	319	15			
2	G	217	Total	C	N	O	S	0	0	0
			1731	1108	288	320	15			
2	H	220	Total	C	N	O	S	0	0	0
			1737	1109	288	325	15			

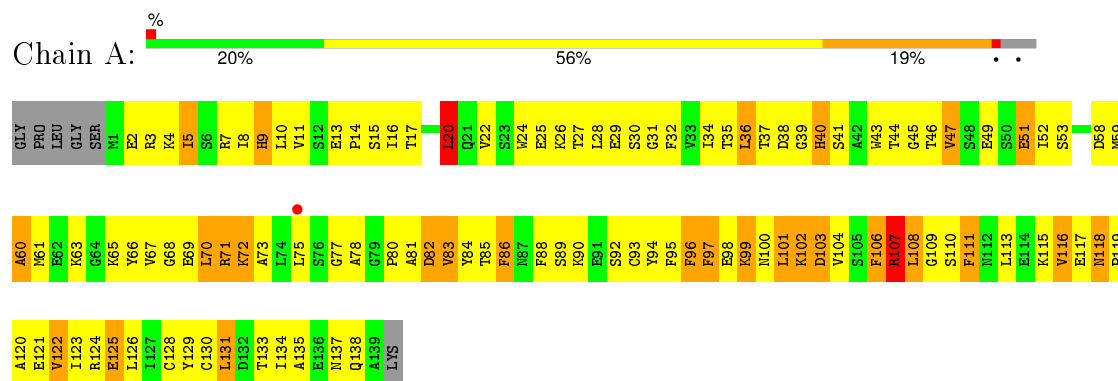
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
C	-3	PRO	-	EXPRESSION TAG	UNP Q9H9Q4
C	-2	LEU	-	EXPRESSION TAG	UNP Q9H9Q4
C	-1	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
C	0	SER	-	EXPRESSION TAG	UNP Q9H9Q4
D	-4	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
D	-3	PRO	-	EXPRESSION TAG	UNP Q9H9Q4
D	-2	LEU	-	EXPRESSION TAG	UNP Q9H9Q4
D	-1	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
D	0	SER	-	EXPRESSION TAG	UNP Q9H9Q4
G	-4	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
G	-3	PRO	-	EXPRESSION TAG	UNP Q9H9Q4
G	-2	LEU	-	EXPRESSION TAG	UNP Q9H9Q4
G	-1	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
G	0	SER	-	EXPRESSION TAG	UNP Q9H9Q4
H	-4	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
H	-3	PRO	-	EXPRESSION TAG	UNP Q9H9Q4
H	-2	LEU	-	EXPRESSION TAG	UNP Q9H9Q4
H	-1	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
H	0	SER	-	EXPRESSION TAG	UNP Q9H9Q4

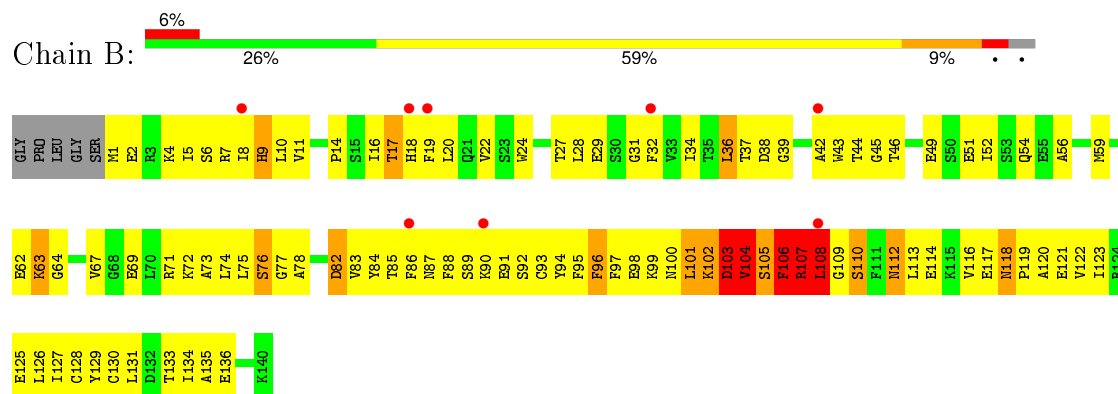
### 3 Residue-property plots [i](#)

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

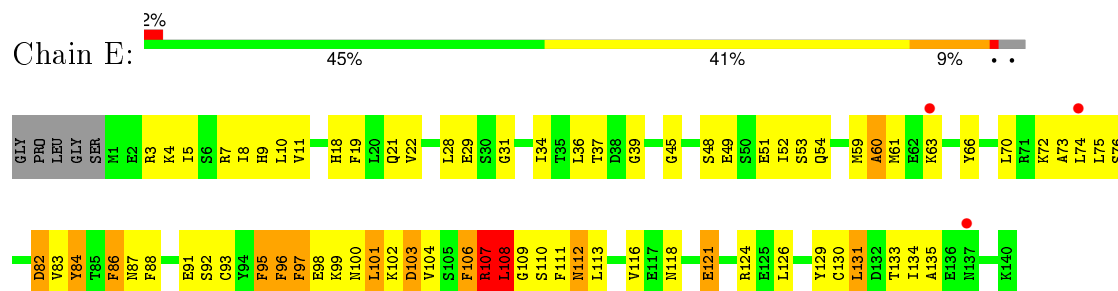
#### • Molecule 1: DNA repair protein XRCC4



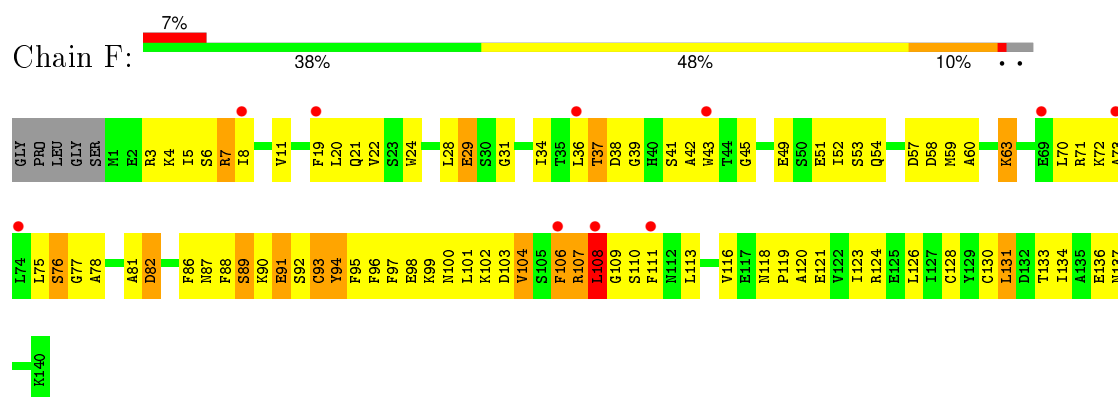
#### • Molecule 1: DNA repair protein XRCC4



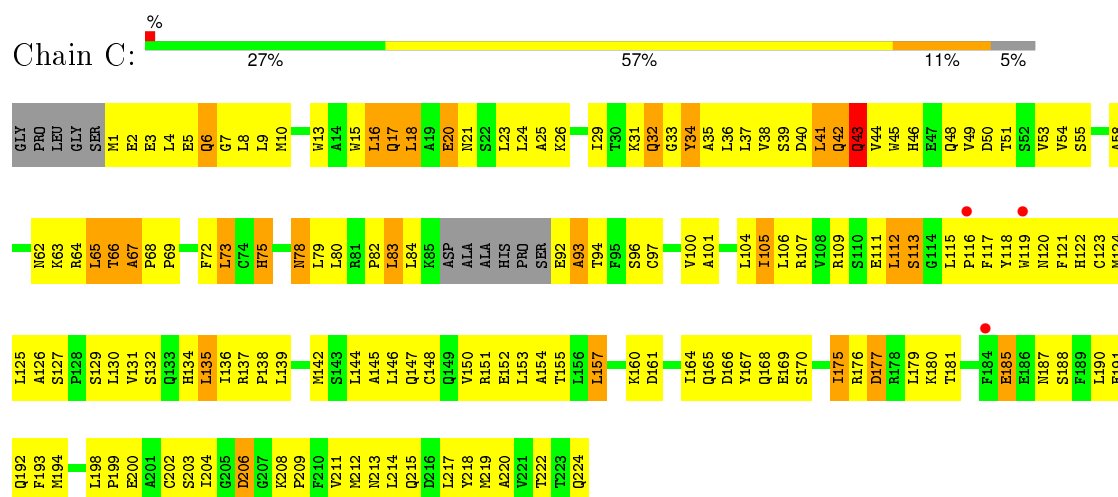
#### • Molecule 1: DNA repair protein XRCC4



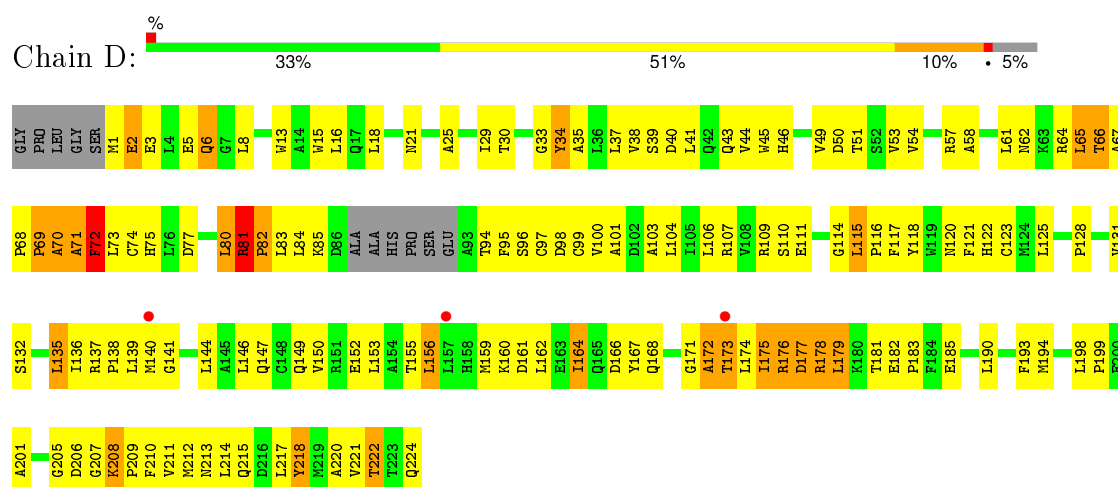
#### • Molecule 1: DNA repair protein XRCC4



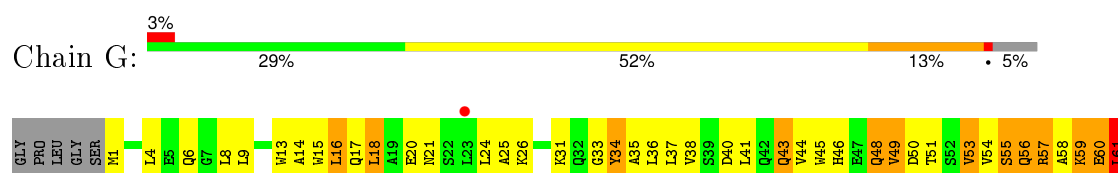
• Molecule 2: Non-homologous end-joining factor 1



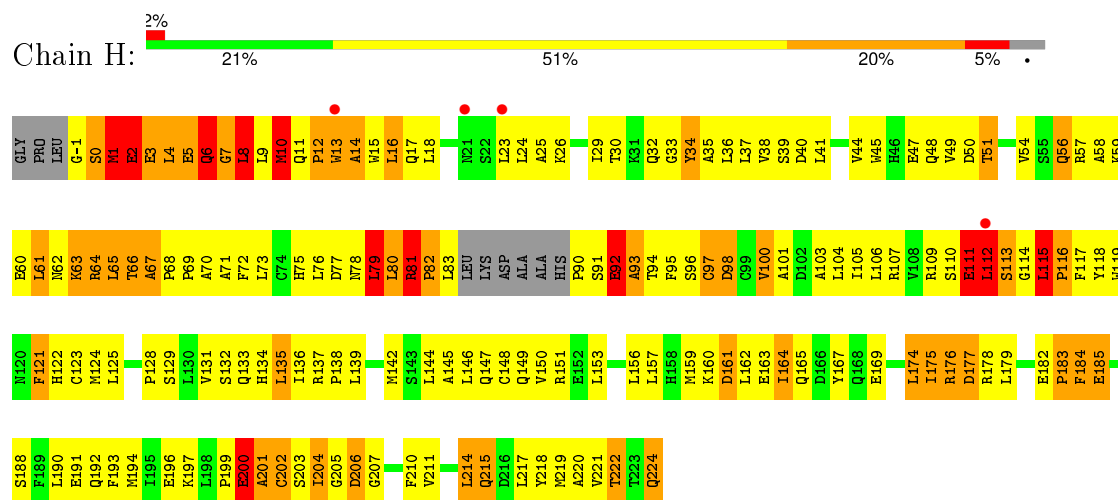
• Molecule 2: Non-homologous end-joining factor 1



• Molecule 2: Non-homologous end-joining factor 1



- Molecule 2: Non-homologous end-joining factor 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.02Å 110.02Å 763.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.44 – 3.97 67.44 – 3.97	Depositor EDS
% Data completeness (in resolution range)	86.5 (67.44-3.97) 86.8 (67.44-3.97)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 4.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.358 , 0.369 0.332 , 0.355	Depositor DCC
$R_{free}$ test set	1701 reflections (7.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	154.4	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	3 of 25102 reflections (0.012%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.77	0/1125	0.97	3/1517 (0.2%)
1	B	0.60	0/1134	0.78	0/1528
1	E	0.36	0/1134	0.53	0/1528
1	F	0.31	0/1134	0.47	0/1528
2	C	0.28	0/1770	0.50	1/2398 (0.0%)
2	D	0.30	0/1754	0.53	1/2379 (0.0%)
2	G	0.35	0/1765	0.58	0/2392
2	H	0.41	0/1772	0.64	2/2402 (0.1%)
All	All	0.43	0/11588	0.63	7/15672 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	81	ARG	C-N-CD	-7.42	104.28	120.60
1	A	20	LEU	CA-CB-CG	7.00	131.39	115.30
2	D	81	ARG	C-N-CD	-6.55	106.19	120.60
2	H	115	LEU	CA-CB-CG	6.49	130.22	115.30
2	C	67	ALA	N-CA-CB	-5.53	102.36	110.10
1	A	20	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	A	20	LEU	CB-CG-CD1	5.04	119.57	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	1103	0	1075	180	0
1	B	1112	0	1088	204	0
1	E	1112	0	1088	107	0
1	F	1112	0	1088	108	0
2	C	1736	0	1752	234	0
2	D	1720	0	1712	182	0
2	G	1731	0	1743	209	0
2	H	1737	0	1733	278	0
All	All	11363	0	11279	1323	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 58.

All (1323) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:HG22	1:B:134:ILE:CG1	1.37	1.50
2:H:8:LEU:CD1	2:H:26:LYS:HD2	1.39	1.49
1:B:107:ARG:NH1	2:C:64:ARG:HD2	1.31	1.43
1:E:134:ILE:HG22	1:F:134:ILE:CG1	1.48	1.42
1:A:134:ILE:CG2	1:B:134:ILE:HD11	1.51	1.40
2:H:8:LEU:HD11	2:H:26:LYS:CD	1.58	1.34
2:H:79:LEU:HD12	2:H:79:LEU:C	1.53	1.25
2:H:80:LEU:H	2:H:80:LEU:CD2	1.49	1.20
1:A:134:ILE:CG2	1:B:134:ILE:CD1	2.19	1.19
1:E:134:ILE:CG2	1:F:134:ILE:CG1	2.20	1.19
1:B:107:ARG:NH1	2:C:64:ARG:CD	2.07	1.17
2:H:80:LEU:N	2:H:80:LEU:HD23	1.57	1.17
2:H:8:LEU:CD1	2:H:26:LYS:CD	2.20	1.16
1:B:104:VAL:CG1	2:C:67:ALA:CB	2.23	1.16
1:A:134:ILE:HG22	1:B:134:ILE:CD1	1.76	1.12
1:E:98:GLU:HA	1:E:107:ARG:O	1.49	1.12
2:H:8:LEU:C	2:H:8:LEU:HD12	1.67	1.11
1:B:104:VAL:CG1	2:C:67:ALA:HB2	1.81	1.11
1:A:134:ILE:CG2	1:B:134:ILE:CG1	2.30	1.10
2:H:8:LEU:O	2:H:8:LEU:HD12	1.52	1.10
1:E:107:ARG:HG2	1:E:107:ARG:HH11	1.06	1.10
2:C:83:LEU:HG	2:C:84:LEU:HD12	1.25	1.10
2:H:8:LEU:O	2:H:11:GLN:HB3	1.53	1.08
1:A:107:ARG:HG2	1:A:108:LEU:H	1.18	1.08
2:H:112:LEU:HG	2:H:112:LEU:O	1.50	1.08
2:G:54:VAL:O	2:G:58:ALA:HB2	1.52	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:HD2	1:B:106:PHE:N	1.52	1.07
1:A:134:ILE:HG22	1:B:134:ILE:HG12	1.30	1.07
1:E:134:ILE:HG22	1:F:134:ILE:HG12	1.08	1.06
1:E:134:ILE:HG22	1:F:134:ILE:HG13	1.37	1.05
1:E:134:ILE:HG23	1:F:134:ILE:HD11	1.30	1.04
1:A:61:MET:HB3	1:A:65:LYS:HD3	1.40	1.03
2:H:79:LEU:HD12	2:H:79:LEU:O	1.57	1.03
2:C:78:ASN:O	2:C:82:PRO:HD3	1.57	1.03
1:A:134:ILE:HG22	1:B:134:ILE:HG13	1.34	1.03
1:E:95:PHE:O	1:E:95:PHE:HD2	1.41	1.03
2:C:125:LEU:HD11	2:D:128:PRO:HG2	1.40	1.02
1:B:104:VAL:HG13	2:C:67:ALA:HB1	1.42	1.02
1:F:104:VAL:HB	1:F:106:PHE:HE2	1.19	1.01
2:G:54:VAL:O	2:G:58:ALA:CB	2.09	1.01
2:G:199:PRO:HA	2:H:224:GLN:HE22	1.22	1.01
1:B:106:PHE:CD2	1:B:106:PHE:N	2.24	1.01
2:G:164:ILE:HG23	2:H:164:ILE:HG12	1.42	1.00
2:G:179:LEU:HD23	2:H:162:LEU:HB3	1.42	1.00
2:G:181:THR:HG21	2:H:159:MET:HB3	1.43	1.00
1:B:96:PHE:HZ	2:H:-1:GLY:HA2	1.24	0.99
1:A:118:ASN:HB3	1:A:121:GLU:HG2	1.45	0.98
2:H:161:ASP:OD2	2:H:184:PHE:HB3	1.64	0.98
2:H:182:GLU:HG3	2:H:183:PRO:HD2	1.46	0.97
2:D:211:VAL:O	2:D:215:GLN:CB	2.13	0.96
2:D:174:LEU:HG	2:D:175:ILE:H	1.30	0.96
2:H:82:PRO:HG3	2:H:90:PRO:HD2	1.46	0.96
2:H:67:ALA:HB1	2:H:68:PRO:HD2	1.46	0.96
2:H:79:LEU:CD1	2:H:79:LEU:C	2.29	0.95
1:E:95:PHE:C	1:E:95:PHE:CD2	2.38	0.95
1:F:107:ARG:HG2	1:F:108:LEU:H	1.29	0.95
1:F:20:LEU:HD11	1:F:36:LEU:HD12	1.48	0.95
2:G:81:ARG:HB3	2:G:82:PRO:HD3	1.47	0.95
1:E:134:ILE:CG2	1:F:134:ILE:HG12	1.92	0.95
2:H:-1:GLY:O	2:H:1:MET:N	1.99	0.94
2:C:41:LEU:O	2:C:42:GLN:HB2	1.68	0.94
1:A:134:ILE:HG23	1:B:134:ILE:HD11	0.94	0.94
2:D:58:ALA:HB1	2:D:72:PHE:CZ	2.03	0.93
2:H:16:LEU:HD13	2:H:17:GLN:H	1.31	0.93
1:B:103:ASP:HA	1:B:104:VAL:C	1.88	0.93
1:E:98:GLU:HB2	1:E:107:ARG:HA	1.49	0.92
1:E:95:PHE:C	1:E:95:PHE:HD2	1.72	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ARG:HH11	2:C:64:ARG:HD2	0.83	0.92
1:B:103:ASP:HB3	1:B:104:VAL:O	1.70	0.92
2:C:15:TRP:HE1	2:C:206:ASP:HB2	1.34	0.91
2:H:5:GLU:O	2:H:6:GLN:C	2.07	0.91
2:C:16:LEU:HD21	2:C:83:LEU:HD21	1.50	0.91
2:D:64:ARG:HB2	2:D:65:LEU:HD13	1.53	0.90
2:H:5:GLU:O	2:H:8:LEU:HB3	1.71	0.90
1:A:134:ILE:HG23	1:B:134:ILE:CD1	1.88	0.90
2:D:211:VAL:O	2:D:215:GLN:HB3	1.71	0.90
1:B:99:LYS:HB2	1:B:108:LEU:HD23	1.51	0.90
1:E:134:ILE:HG23	1:F:134:ILE:CD1	2.02	0.90
2:D:54:VAL:O	2:D:58:ALA:HB2	1.71	0.90
1:B:104:VAL:HG12	2:C:67:ALA:HB2	1.54	0.90
1:E:134:ILE:CG2	1:F:134:ILE:HG13	1.96	0.89
2:C:15:TRP:NE1	2:C:206:ASP:HB2	1.87	0.89
2:C:135:LEU:HB3	2:C:136:ILE:HD12	1.54	0.89
2:C:79:LEU:HD21	2:C:93:ALA:HB2	1.52	0.89
1:B:103:ASP:HA	1:B:104:VAL:O	1.70	0.89
1:F:104:VAL:HB	1:F:106:PHE:CE2	2.07	0.89
2:H:7:GLY:O	2:H:9:LEU:N	2.07	0.88
1:B:104:VAL:HG12	2:C:67:ALA:CB	1.99	0.88
2:H:80:LEU:H	2:H:80:LEU:HD23	0.73	0.88
2:H:67:ALA:HB1	2:H:68:PRO:CD	2.04	0.88
2:D:37:LEU:HD12	2:D:46:HIS:HB2	1.55	0.88
2:D:103:ALA:HA	2:D:123:CYS:O	1.74	0.87
1:B:107:ARG:HH11	2:C:64:ARG:CD	1.76	0.87
1:E:107:ARG:HG2	1:E:107:ARG:NH1	1.84	0.87
2:C:147:GLN:O	2:C:151:ARG:HG2	1.74	0.87
1:B:94:TYR:HD1	1:B:112:ASN:HD22	1.23	0.87
2:H:5:GLU:O	2:H:6:GLN:O	1.92	0.87
2:H:9:LEU:C	2:H:11:GLN:H	1.75	0.87
1:A:32:PHE:O	1:A:47:VAL:HG23	1.75	0.87
1:B:104:VAL:HG13	2:C:67:ALA:CB	1.97	0.87
1:A:107:ARG:HG2	1:A:108:LEU:N	1.87	0.87
1:F:98:GLU:HA	1:F:107:ARG:HA	1.54	0.87
1:E:106:PHE:O	1:E:107:ARG:HB3	1.75	0.86
2:C:79:LEU:O	2:C:82:PRO:HD2	1.75	0.86
2:C:42:GLN:O	2:C:43:GLN:HB2	1.74	0.86
1:B:86:PHE:HD1	1:B:95:PHE:HZ	1.20	0.86
1:E:98:GLU:CB	1:E:107:ARG:HA	2.05	0.85
1:A:98:GLU:HA	1:A:107:ARG:HA	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:TRP:CD1	1:A:115:LYS:HB2	2.11	0.85
1:E:95:PHE:CD2	1:E:95:PHE:O	2.30	0.85
1:F:51:GLU:HA	1:F:54:GLN:HB3	1.59	0.84
2:H:8:LEU:HD12	2:H:26:LYS:HD2	1.57	0.84
2:G:54:VAL:HG11	2:G:73:LEU:HD21	1.59	0.84
1:E:107:ARG:HH11	1:E:107:ARG:CG	1.90	0.83
1:A:82:ASP:HA	1:A:101:LEU:HD11	1.58	0.83
2:G:16:LEU:HD13	2:G:17:GLN:H	1.42	0.83
2:G:157:LEU:HG	2:H:157:LEU:HG	1.57	0.83
2:G:107:ARG:NH1	2:G:120:ASN:HD21	1.77	0.83
2:G:94:THR:HG21	2:G:109:ARG:HH11	1.43	0.83
1:B:107:ARG:HH12	2:C:64:ARG:CD	1.88	0.83
2:H:13:TRP:O	2:H:14:ALA:HB2	1.77	0.83
1:E:87:ASN:HB2	1:E:96:PHE:CE1	2.14	0.83
2:G:75:HIS:CE1	2:G:117:PHE:HD2	1.97	0.83
2:H:44:VAL:O	2:H:125:LEU:HD12	1.79	0.82
1:B:8:ILE:HG21	1:B:20:LEU:HD22	1.61	0.82
2:G:199:PRO:HA	2:H:224:GLN:NE2	1.94	0.82
2:D:175:ILE:HG22	2:D:176:ARG:HG2	1.61	0.82
2:G:201:ALA:HB1	2:H:145:ALA:HA	1.61	0.82
2:C:165:GLN:O	2:C:169:GLU:HG2	1.81	0.81
1:B:72:LYS:HB3	1:B:78:ALA:HA	1.61	0.81
2:D:58:ALA:HB1	2:D:72:PHE:HZ	1.46	0.81
2:C:34:TYR:CE1	2:C:49:VAL:HB	2.15	0.81
1:A:99:LYS:HG3	1:A:100:ASN:N	1.95	0.81
2:G:118:TYR:C	2:G:118:TYR:HD2	1.84	0.81
1:B:103:ASP:CA	1:B:104:VAL:O	2.29	0.80
2:H:92:GLU:O	2:H:93:ALA:CB	2.28	0.80
1:B:96:PHE:HZ	2:H:-1:GLY:CA	1.93	0.80
2:G:62:ASN:ND2	2:G:117:PHE:HD1	1.79	0.80
2:D:211:VAL:O	2:D:215:GLN:HB2	1.81	0.80
1:E:22:VAL:HG22	1:E:34:ILE:HG13	1.63	0.80
1:F:88:PHE:HD1	1:F:95:PHE:HB2	1.46	0.80
1:B:102:LYS:CD	1:B:102:LYS:O	2.30	0.80
2:H:115:LEU:O	2:H:116:PRO:O	1.99	0.80
2:H:80:LEU:O	2:H:81:ARG:CB	2.30	0.80
1:A:107:ARG:CG	1:A:108:LEU:H	1.95	0.80
2:C:204:ILE:HG23	2:D:140:MET:SD	2.22	0.79
2:C:167:TYR:CE1	2:D:174:LEU:HD13	2.18	0.79
2:H:112:LEU:HD22	2:H:117:PHE:HD1	1.47	0.79
2:G:8:LEU:HD22	2:G:35:ALA:HB1	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:TRP:HE1	2:H:121:PHE:HA	1.46	0.79
1:A:37:THR:HG22	1:A:39:GLY:H	1.46	0.79
2:G:162:LEU:HB3	2:H:179:LEU:HD23	1.65	0.79
1:B:103:ASP:CB	1:B:104:VAL:O	2.30	0.79
2:H:8:LEU:O	2:H:11:GLN:CB	2.30	0.79
1:B:106:PHE:HD1	2:C:115:LEU:HD12	1.46	0.79
2:H:-1:GLY:N	2:H:32:GLN:NE2	2.30	0.79
2:H:79:LEU:CD1	2:H:79:LEU:O	2.30	0.79
1:F:8:ILE:HG21	1:F:20:LEU:HD22	1.65	0.79
2:G:57:ARG:HG2	2:G:57:ARG:HH11	1.48	0.79
2:H:79:LEU:HD12	2:H:80:LEU:N	1.99	0.78
1:F:106:PHE:O	1:F:107:ARG:HB2	1.82	0.77
2:C:78:ASN:O	2:C:82:PRO:CD	2.31	0.77
2:G:137:ARG:HB2	2:G:138:PRO:HD3	1.66	0.77
2:D:65:LEU:HD13	2:D:65:LEU:N	1.98	0.77
2:H:113:SER:O	2:H:115:LEU:N	2.17	0.77
1:B:106:PHE:H	1:B:106:PHE:HD2	1.14	0.77
2:G:109:ARG:HA	2:G:118:TYR:HB2	1.66	0.77
2:C:106:LEU:HB3	2:C:121:PHE:HB2	1.67	0.77
2:C:219:MET:HA	2:C:222:THR:HG22	1.66	0.77
2:G:118:TYR:CD2	2:G:118:TYR:C	2.59	0.77
2:H:112:LEU:HD22	2:H:117:PHE:CD1	2.20	0.76
2:D:69:PRO:O	2:D:72:PHE:HB2	1.86	0.76
2:G:169:GLU:HG3	2:G:170:SER:H	1.50	0.76
1:B:92:SER:O	1:B:94:TYR:N	2.18	0.76
1:E:134:ILE:CG2	1:F:134:ILE:CD1	2.60	0.76
1:E:37:THR:HG22	1:E:39:GLY:H	1.49	0.76
2:H:9:LEU:CD2	2:H:134:HIS:CD2	2.69	0.76
2:H:82:PRO:O	2:H:83:LEU:CB	2.30	0.76
1:A:43:TRP:NE1	1:A:115:LYS:HD3	2.01	0.76
1:E:134:ILE:CG2	1:F:134:ILE:HD11	2.13	0.75
2:G:163:GLU:CD	2:H:164:ILE:HG21	2.05	0.75
1:A:118:ASN:O	1:A:119:PRO:C	2.23	0.75
2:G:131:VAL:O	2:G:135:LEU:HB2	1.86	0.75
1:E:107:ARG:HG3	1:E:108:LEU:N	2.00	0.75
1:A:92:SER:O	1:A:93:CYS:HB2	1.85	0.75
2:D:174:LEU:HD11	2:D:179:LEU:HD11	1.69	0.75
1:E:88:PHE:HD1	1:E:95:PHE:HB2	1.52	0.74
2:G:78:ASN:O	2:G:82:PRO:HD2	1.86	0.74
1:F:133:THR:O	1:F:137:ASN:HB2	1.87	0.74
1:E:107:ARG:O	1:E:108:LEU:HB2	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:ARG:CG	2:G:57:ARG:HH11	2.00	0.74
1:A:93:CYS:HB3	1:A:113:LEU:O	1.88	0.74
1:B:94:TYR:CD1	1:B:112:ASN:ND2	2.56	0.74
1:B:99:LYS:CB	1:B:108:LEU:HD23	2.17	0.74
2:C:18:LEU:HD23	2:C:97:CYS:HB3	1.70	0.74
2:H:-1:GLY:H3	2:H:32:GLN:NE2	1.84	0.73
1:E:133:THR:CG2	1:F:134:ILE:HD13	2.17	0.73
1:B:106:PHE:HD1	2:C:115:LEU:CD1	2.00	0.73
1:B:107:ARG:O	1:B:108:LEU:HB2	1.87	0.73
2:C:18:LEU:HD22	2:C:21:ASN:O	1.88	0.73
2:H:111:GLU:O	2:H:112:LEU:HB3	1.87	0.73
2:C:16:LEU:CD1	2:C:17:GLN:H	2.01	0.73
2:C:16:LEU:HD13	2:C:17:GLN:H	1.53	0.73
2:H:65:LEU:H	2:H:65:LEU:HD22	1.53	0.73
2:G:106:LEU:HB3	2:G:121:PHE:HB2	1.71	0.73
2:H:96:SER:O	2:H:106:LEU:HD12	1.89	0.73
2:D:210:PHE:O	2:D:214:LEU:HB2	1.88	0.72
2:G:169:GLU:HG3	2:G:170:SER:N	2.04	0.72
1:A:32:PHE:CE1	1:A:47:VAL:HG21	2.23	0.72
2:C:45:TRP:CE3	2:C:104:LEU:HD12	2.24	0.72
2:H:9:LEU:C	2:H:11:GLN:N	2.42	0.72
2:G:62:ASN:HD21	2:G:117:PHE:HA	1.52	0.72
2:D:54:VAL:O	2:D:58:ALA:CB	2.36	0.72
1:E:5:ILE:HG12	1:E:21:GLN:HG3	1.71	0.72
2:G:57:ARG:NH1	2:G:57:ARG:HB3	2.04	0.72
2:C:9:LEU:HD23	2:C:134:HIS:CE1	2.24	0.72
2:G:75:HIS:HE1	2:G:117:PHE:HD2	1.33	0.72
2:G:164:ILE:CG2	2:H:164:ILE:HG12	2.19	0.72
1:B:94:TYR:CE2	1:B:110:SER:HB2	2.24	0.72
2:C:58:ALA:HB1	2:C:72:PHE:CZ	2.25	0.71
2:C:167:TYR:HE1	2:D:174:LEU:HD13	1.52	0.71
2:D:62:ASN:HB3	2:D:65:LEU:HD22	1.72	0.71
2:H:211:VAL:HA	2:H:215:GLN:NE2	2.05	0.71
1:B:104:VAL:HG12	2:C:67:ALA:CA	2.19	0.71
1:B:104:VAL:HG11	2:C:67:ALA:HB2	1.72	0.71
2:H:-1:GLY:N	2:H:32:GLN:HE22	1.88	0.71
1:A:99:LYS:CE	1:A:101:LEU:HD13	2.21	0.71
2:H:4:LEU:O	2:H:5:GLU:C	2.29	0.71
2:G:167:TYR:HD2	2:H:167:TYR:HB3	1.53	0.71
2:G:170:SER:HB3	2:H:175:ILE:HD12	1.72	0.71
2:H:185:GLU:HA	2:H:185:GLU:OE2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:HD1	1:B:112:ASN:ND2	1.88	0.71
2:H:9:LEU:O	2:H:11:GLN:N	2.23	0.71
1:F:88:PHE:CD1	1:F:95:PHE:HB2	2.25	0.71
2:H:8:LEU:HD11	2:H:26:LYS:HD2	0.72	0.71
2:G:167:TYR:CD2	2:H:167:TYR:HB3	2.25	0.71
1:B:5:ILE:HG22	1:B:6:SER:H	1.54	0.71
2:C:31:LYS:O	2:C:32:GLN:HB2	1.89	0.71
2:H:6:GLN:O	2:H:7:GLY:C	2.29	0.70
2:H:7:GLY:O	2:H:8:LEU:C	2.29	0.70
2:H:160:LYS:O	2:H:164:ILE:HG13	1.91	0.70
2:C:164:ILE:HD11	2:D:160:LYS:HB3	1.71	0.70
2:G:131:VAL:HA	2:G:135:LEU:HD23	1.73	0.70
2:C:165:GLN:HA	2:C:168:GLN:HG2	1.73	0.70
2:C:213:ASN:C	2:C:214:LEU:HD23	2.12	0.70
2:C:79:LEU:C	2:C:82:PRO:HD2	2.11	0.70
2:H:2:GLU:O	2:H:3:GLU:C	2.30	0.70
2:C:1:MET:SD	2:C:4:LEU:HD12	2.32	0.70
2:D:211:VAL:HA	2:D:215:GLN:HB2	1.72	0.70
2:G:81:ARG:CB	2:G:82:PRO:HD3	2.20	0.70
2:C:164:ILE:HG12	2:D:164:ILE:HG12	1.74	0.70
1:F:118:ASN:HD22	1:F:121:GLU:H	1.40	0.70
2:H:200:GLU:CG	2:H:201:ALA:H	2.04	0.70
1:A:100:ASN:O	1:A:101:LEU:HD12	1.92	0.70
2:G:93:ALA:CB	2:G:110:SER:HB3	2.22	0.70
1:B:102:LYS:O	1:B:102:LYS:HD3	1.92	0.69
2:G:16:LEU:CD1	2:G:17:GLN:H	2.04	0.69
2:G:144:LEU:HD23	2:H:201:ALA:O	1.92	0.69
1:B:107:ARG:HD2	1:B:108:LEU:H	1.56	0.69
1:F:86:PHE:HB3	1:F:95:PHE:CZ	2.26	0.69
1:B:126:LEU:HD12	1:B:126:LEU:C	2.13	0.69
2:C:194:MET:HA	2:C:198:LEU:HB2	1.74	0.69
2:H:94:THR:HG22	2:H:94:THR:O	1.91	0.69
2:H:7:GLY:O	2:H:10:MET:N	2.25	0.69
1:E:96:PHE:HD1	1:E:96:PHE:O	1.75	0.69
2:D:80:LEU:HB3	2:D:85:LYS:CB	2.22	0.69
2:H:9:LEU:HD23	2:H:134:HIS:CD2	2.29	0.68
2:H:0:SER:O	2:H:1:MET:C	2.30	0.68
2:D:30:THR:O	2:D:73:LEU:HD13	1.92	0.68
2:D:18:LEU:HD13	2:D:97:CYS:HB2	1.75	0.68
2:D:64:ARG:HB2	2:D:65:LEU:CD1	2.22	0.68
1:A:119:PRO:HG2	1:A:120:ALA:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:54:VAL:O	2:H:58:ALA:CB	2.42	0.68
1:B:86:PHE:HD1	1:B:95:PHE:CZ	2.07	0.68
1:B:74:LEU:O	1:B:75:LEU:HD23	1.94	0.68
2:H:137:ARG:HB2	2:H:138:PRO:HD3	1.76	0.68
2:H:8:LEU:HD11	2:H:26:LYS:CG	2.22	0.68
2:H:-1:GLY:H1	2:H:32:GLN:HE22	1.40	0.67
1:E:104:VAL:HB	1:E:106:PHE:CE2	2.29	0.67
2:C:169:GLU:HG3	2:C:170:SER:N	2.09	0.67
2:C:153:LEU:HD11	2:D:150:VAL:HG13	1.76	0.67
1:B:96:PHE:CZ	2:H:0:SER:N	2.62	0.67
2:D:175:ILE:HG22	2:D:176:ARG:N	2.08	0.67
1:B:96:PHE:CZ	2:H:-1:GLY:HA2	2.17	0.67
2:C:80:LEU:O	2:C:84:LEU:HD13	1.93	0.67
2:G:104:LEU:O	2:G:123:CYS:HB2	1.94	0.67
2:D:137:ARG:HB2	2:D:138:PRO:HD3	1.76	0.67
2:D:64:ARG:CB	2:D:65:LEU:HD13	2.25	0.67
1:F:88:PHE:HB2	1:F:95:PHE:HD2	1.59	0.67
1:B:133:THR:O	1:B:134:ILE:C	2.33	0.67
1:A:103:ASP:HA	1:A:104:VAL:CB	2.24	0.67
1:E:133:THR:HG22	1:F:134:ILE:HD13	1.76	0.66
2:H:13:TRP:O	2:H:14:ALA:CB	2.42	0.66
2:H:94:THR:HB	2:H:109:ARG:O	1.95	0.66
2:C:16:LEU:HD12	2:C:18:LEU:CD1	2.25	0.66
1:F:99:LYS:HG2	1:F:100:ASN:N	2.11	0.66
2:H:72:PHE:HA	2:H:75:HIS:HD2	1.59	0.66
2:G:75:HIS:NE2	2:G:112:LEU:HB2	2.09	0.66
2:D:1:MET:O	2:D:3:GLU:N	2.28	0.66
1:B:96:PHE:HB2	1:B:110:SER:HB3	1.78	0.66
2:H:16:LEU:CD1	2:H:17:GLN:H	2.07	0.66
2:C:137:ARG:HB2	2:C:138:PRO:HD3	1.78	0.66
1:A:82:ASP:HB3	1:A:84:TYR:CE2	2.31	0.66
1:F:89:SER:OG	1:F:91:GLU:HG2	1.95	0.66
1:B:118:ASN:HB3	1:B:121:GLU:HB2	1.77	0.66
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.59	0.66
1:A:134:ILE:HG21	1:B:130:CYS:SG	2.36	0.66
2:G:54:VAL:O	2:G:58:ALA:HB3	1.96	0.66
1:A:128:CYS:HG	1:B:19:PHE:HZ	1.44	0.66
2:H:1:MET:O	2:H:3:GLU:N	2.29	0.65
1:B:36:LEU:HD23	1:B:36:LEU:O	1.96	0.65
2:C:8:LEU:HD22	2:C:35:ALA:HB1	1.77	0.65
1:B:37:THR:CG2	1:B:38:ASP:N	2.58	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:HIS:C	2:C:75:HIS:ND1	2.49	0.65
2:C:83:LEU:HG	2:C:84:LEU:CD1	2.14	0.65
1:E:3:ARG:HG2	1:E:4:LYS:N	2.12	0.65
2:C:75:HIS:C	2:C:75:HIS:HD1	2.00	0.65
1:F:102:LYS:O	1:F:103:ASP:HB2	1.96	0.65
2:G:49:VAL:HG13	2:G:50:ASP:N	2.11	0.65
2:H:57:ARG:O	2:H:61:LEU:HD22	1.95	0.65
1:B:106:PHE:O	1:B:107:ARG:HB2	1.94	0.65
2:G:54:VAL:HG23	2:G:69:PRO:HB3	1.77	0.65
1:B:133:THR:O	1:B:135:ALA:N	2.29	0.65
1:A:37:THR:HG22	1:A:38:ASP:N	2.12	0.65
1:B:96:PHE:CZ	2:H:-1:GLY:CA	2.78	0.65
1:E:106:PHE:O	1:E:107:ARG:CB	2.44	0.65
1:E:112:ASN:N	1:E:112:ASN:OD1	2.30	0.65
1:B:102:LYS:O	1:B:103:ASP:C	2.35	0.65
2:H:2:GLU:O	2:H:4:LEU:N	2.30	0.65
1:A:43:TRP:HD1	1:A:115:LYS:HB2	1.62	0.65
1:B:103:ASP:CA	1:B:104:VAL:C	2.64	0.65
2:H:24:LEU:HD11	2:H:207:GLY:HA3	1.79	0.65
1:A:25:GLU:OE2	1:A:30:SER:HB3	1.96	0.65
2:H:0:SER:O	2:H:2:GLU:N	2.30	0.65
2:D:45:TRP:HB3	2:D:123:CYS:HB3	1.78	0.65
1:E:34:ILE:HG21	1:E:111:PHE:HE1	1.61	0.65
1:F:11:VAL:O	1:F:11:VAL:HG12	1.97	0.65
2:D:74:CYS:O	2:D:77:ASP:HB3	1.96	0.65
2:H:161:ASP:OD2	2:H:184:PHE:CB	2.43	0.65
2:H:92:GLU:O	2:H:93:ALA:HB2	1.97	0.64
2:H:18:LEU:CD2	2:H:95:PHE:HB3	2.27	0.64
2:H:66:THR:O	2:H:67:ALA:HB2	1.98	0.64
1:F:11:VAL:HB	1:F:87:ASN:OD1	1.97	0.64
2:G:75:HIS:CE1	2:G:117:PHE:CD2	2.84	0.64
2:H:131:VAL:O	2:H:135:LEU:HB3	1.97	0.64
2:D:74:CYS:O	2:D:77:ASP:CB	2.46	0.64
1:E:53:SER:HA	1:E:63:LYS:HD3	1.79	0.64
2:H:2:GLU:O	2:H:5:GLU:N	2.30	0.64
1:B:20:LEU:HD12	1:B:36:LEU:HB2	1.78	0.64
2:H:56:GLN:HG2	2:H:57:ARG:N	2.11	0.64
2:G:142:MET:HE1	2:G:214:LEU:HB3	1.79	0.64
1:B:107:ARG:HG3	2:C:64:ARG:HB3	1.79	0.64
1:A:66:TYR:CE1	1:A:108:LEU:HD23	2.33	0.64
1:F:6:SER:CB	1:F:76:SER:HB2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TYR:CD1	1:B:97:PHE:HZ	2.16	0.64
2:H:97:CYS:HB2	2:H:106:LEU:HD13	1.80	0.64
1:A:106:PHE:O	1:A:107:ARG:HB3	1.96	0.64
2:D:174:LEU:HG	2:D:175:ILE:N	2.08	0.64
1:B:86:PHE:CD1	1:B:95:PHE:HZ	2.09	0.64
1:E:66:TYR:HE1	1:E:108:LEU:HD23	1.64	0.63
2:C:125:LEU:HD11	2:D:128:PRO:CG	2.21	0.63
1:F:98:GLU:CA	1:F:107:ARG:HA	2.27	0.63
2:D:15:TRP:C	2:D:16:LEU:HD12	2.18	0.63
2:D:6:GLN:HE21	2:D:6:GLN:HA	1.63	0.63
2:G:194:MET:HA	2:G:198:LEU:HB2	1.81	0.63
1:E:87:ASN:HB2	1:E:96:PHE:HE1	1.62	0.63
2:G:166:ASP:OD2	2:H:174:LEU:HD12	1.99	0.63
2:H:40:ASP:O	2:H:41:LEU:HB2	1.99	0.63
2:H:8:LEU:CD1	2:H:26:LYS:CG	2.76	0.63
2:G:199:PRO:CA	2:H:224:GLN:HE22	2.04	0.63
2:C:213:ASN:O	2:C:214:LEU:HD23	1.99	0.63
1:B:136:GLU:O	1:B:136:GLU:HG3	1.99	0.63
1:A:25:GLU:CD	1:A:30:SER:HB3	2.19	0.63
2:D:176:ARG:HB3	2:D:178:ARG:HH21	1.62	0.63
1:F:88:PHE:HB2	1:F:95:PHE:CD2	2.34	0.63
2:H:119:TRP:HE1	2:H:121:PHE:CA	2.10	0.63
2:H:80:LEU:N	2:H:80:LEU:CD2	2.30	0.63
1:B:37:THR:HG22	1:B:38:ASP:N	2.14	0.62
1:A:4:LYS:HG2	1:A:5:ILE:H	1.64	0.62
1:E:99:LYS:O	1:E:106:PHE:HB2	1.98	0.62
2:H:50:ASP:O	2:H:54:VAL:HG23	1.99	0.62
1:F:6:SER:HB2	1:F:76:SER:HB2	1.82	0.62
2:G:146:LEU:HB3	2:H:146:LEU:HB3	1.81	0.62
2:G:181:THR:CG2	2:H:159:MET:HB3	2.23	0.62
2:D:50:ASP:O	2:D:54:VAL:HG23	1.98	0.62
1:B:5:ILE:HG22	1:B:6:SER:N	2.13	0.62
1:E:59:MET:O	1:E:60:ALA:HB3	1.99	0.62
1:A:82:ASP:HA	1:A:101:LEU:CD1	2.29	0.62
1:A:106:PHE:O	1:A:107:ARG:CB	2.47	0.62
1:A:124:ARG:CZ	1:B:16:ILE:HG23	2.29	0.62
2:G:119:TRP:CD1	2:G:121:PHE:CD1	2.87	0.62
1:F:37:THR:OG1	1:F:42:ALA:HA	2.00	0.62
1:A:4:LYS:CG	1:A:5:ILE:H	2.13	0.62
2:H:8:LEU:C	2:H:8:LEU:CD1	2.43	0.62
1:F:72:LYS:HG2	1:F:77:GLY:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:PHE:HD2	2:H:214:LEU:HD12	1.64	0.62
2:H:82:PRO:CG	2:H:90:PRO:HD2	2.26	0.62
2:C:160:LYS:O	2:C:164:ILE:HG13	2.00	0.62
2:G:105:ILE:HD13	2:G:120:ASN:HD22	1.64	0.62
1:A:96:PHE:HB2	1:A:109:GLY:O	2.00	0.62
1:E:19:PHE:HZ	1:F:128:CYS:HG	1.48	0.62
2:H:103:ALA:HA	2:H:123:CYS:O	1.99	0.62
1:B:133:THR:HG22	1:B:134:ILE:N	2.14	0.61
2:C:105:ILE:CD1	2:G:101:ALA:H	2.13	0.61
1:A:4:LYS:HG2	1:A:5:ILE:N	2.15	0.61
2:D:178:ARG:HG2	2:D:179:LEU:N	2.15	0.61
1:F:92:SER:O	1:F:94:TYR:N	2.31	0.61
2:G:107:ARG:CZ	2:G:120:ASN:HD21	2.13	0.61
2:H:211:VAL:HA	2:H:215:GLN:HE21	1.65	0.61
2:H:59:LYS:HE2	2:H:66:THR:HB	1.81	0.61
2:H:54:VAL:O	2:H:58:ALA:HB2	2.00	0.61
2:H:5:GLU:O	2:H:8:LEU:N	2.33	0.61
1:A:99:LYS:HB3	1:A:108:LEU:HD12	1.81	0.61
2:H:75:HIS:O	2:H:78:ASN:HB2	2.01	0.61
2:H:2:GLU:O	2:H:4:LEU:C	2.40	0.60
2:G:119:TRP:HE1	2:G:121:PHE:CA	2.14	0.60
2:H:200:GLU:HG2	2:H:201:ALA:N	2.16	0.60
1:B:27:THR:HG23	1:B:71:ARG:HH22	1.66	0.60
1:A:68:GLY:O	1:A:72:LYS:HG3	2.01	0.60
2:G:111:GLU:O	2:G:112:LEU:HB3	2.01	0.60
2:G:94:THR:CG2	2:G:109:ARG:HH11	2.11	0.60
2:H:200:GLU:CG	2:H:201:ALA:N	2.64	0.60
1:A:99:LYS:HD2	1:A:101:LEU:HD13	1.83	0.60
1:A:35:THR:HG23	1:A:44:THR:HG1	1.65	0.60
1:B:104:VAL:CG1	2:C:67:ALA:HB1	2.06	0.60
1:E:66:TYR:CE1	1:E:108:LEU:HD23	2.35	0.60
2:H:109:ARG:HG3	2:H:118:TYR:CE2	2.36	0.60
2:C:170:SER:HB3	2:D:175:ILE:HD12	1.83	0.60
1:A:53:SER:HA	1:A:63:LYS:HD3	1.83	0.60
1:A:117:GLU:O	1:A:119:PRO:HD2	2.00	0.60
2:D:75:HIS:CE1	2:D:117:PHE:HD2	2.19	0.60
1:F:24:TRP:CH2	1:F:75:LEU:HD11	2.36	0.60
2:H:8:LEU:HD12	2:H:26:LYS:CD	2.23	0.60
2:G:62:ASN:ND2	2:G:117:PHE:HA	2.16	0.60
2:G:36:LEU:HD22	2:G:121:PHE:CD2	2.36	0.60
2:D:176:ARG:HB2	2:D:179:LEU:HG	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:O	1:B:78:ALA:HB2	2.00	0.60
1:B:63:LYS:NZ	1:B:63:LYS:H	2.00	0.60
1:A:134:ILE:CG2	1:B:134:ILE:HG13	2.16	0.60
1:E:100:ASN:O	1:E:101:LEU:HD23	2.01	0.60
2:C:49:VAL:HG13	2:C:53:VAL:HG13	1.83	0.60
2:D:144:LEU:O	2:D:147:GLN:HB3	2.02	0.60
2:D:33:GLY:HA3	2:D:49:VAL:O	2.01	0.60
2:D:39:SER:HB2	2:D:44:VAL:HG22	1.84	0.60
1:B:99:LYS:HG2	1:B:100:ASN:N	2.16	0.60
2:C:23:LEU:HD11	2:C:97:CYS:SG	2.41	0.60
2:H:38:VAL:HG12	2:H:39:SER:H	1.67	0.60
2:C:62:ASN:HB3	2:C:65:LEU:HB2	1.83	0.59
2:H:9:LEU:HD21	2:H:134:HIS:NE2	2.16	0.59
2:G:75:HIS:CE1	2:G:112:LEU:HB2	2.37	0.59
2:G:18:LEU:HB3	2:G:95:PHE:HB2	1.83	0.59
2:C:34:TYR:O	2:C:34:TYR:HD1	1.84	0.59
2:D:107:ARG:HG2	2:D:120:ASN:CB	2.32	0.59
2:H:9:LEU:CD2	2:H:134:HIS:NE2	2.65	0.59
1:F:107:ARG:HB3	2:G:64:ARG:HB3	1.84	0.59
2:C:175:ILE:HG12	2:D:167:TYR:OH	2.01	0.59
1:A:28:LEU:HD11	1:A:32:PHE:CD2	2.38	0.59
2:C:8:LEU:HD11	2:C:26:LYS:HG3	1.85	0.59
1:F:59:MET:O	1:F:60:ALA:HB3	2.03	0.59
1:F:5:ILE:HG12	1:F:21:GLN:HG3	1.83	0.59
2:G:13:TRP:CZ2	2:G:26:LYS:HE3	2.38	0.59
2:G:175:ILE:HD12	2:G:180:LYS:HB2	1.84	0.59
1:B:75:LEU:O	1:B:77:GLY:N	2.36	0.59
1:F:82:ASP:HA	1:F:101:LEU:HD21	1.83	0.59
2:G:182:GLU:HG3	2:G:183:PRO:HD2	1.84	0.59
2:H:144:LEU:O	2:H:147:GLN:HB3	2.02	0.59
2:H:18:LEU:HD13	2:H:97:CYS:HB3	1.84	0.59
1:B:84:TYR:HD1	1:B:97:PHE:HZ	1.49	0.59
2:G:165:GLN:O	2:G:169:GLU:HG2	2.03	0.59
2:C:50:ASP:O	2:C:54:VAL:HG23	2.02	0.59
2:H:-1:GLY:C	2:H:1:MET:N	2.54	0.59
1:A:43:TRP:HE1	1:A:115:LYS:HD3	1.67	0.59
2:G:119:TRP:HE1	2:G:121:PHE:HA	1.67	0.59
1:B:22:VAL:HG22	1:B:34:ILE:HG13	1.82	0.59
1:A:3:ARG:HG3	1:A:129:TYR:OH	2.03	0.59
1:A:22:VAL:HG22	1:A:34:ILE:HG13	1.84	0.59
2:H:-1:GLY:O	2:H:0:SER:C	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:94:THR:HG23	2:G:95:PHE:N	2.17	0.59
2:G:8:LEU:HD22	2:G:35:ALA:CB	2.33	0.59
1:A:17:THR:O	1:A:17:THR:HG22	2.01	0.59
2:H:30:THR:O	2:H:73:LEU:HD13	2.02	0.59
1:A:28:LEU:CD1	1:A:32:PHE:CD2	2.86	0.58
1:B:101:LEU:O	1:B:102:LYS:HB3	2.03	0.58
1:A:99:LYS:CD	1:A:101:LEU:HD13	2.33	0.58
2:H:33:GLY:HA3	2:H:49:VAL:O	2.04	0.58
2:G:175:ILE:HB	2:G:177:ASP:H	1.68	0.58
1:B:102:LYS:HD2	1:B:102:LYS:O	2.03	0.58
2:H:96:SER:OG	2:H:107:ARG:HB2	2.03	0.58
2:H:79:LEU:CG	2:H:79:LEU:O	2.50	0.58
2:D:18:LEU:HD13	2:D:97:CYS:CB	2.33	0.58
1:F:22:VAL:HG22	1:F:34:ILE:HG13	1.85	0.58
1:B:86:PHE:HB3	1:B:95:PHE:HE2	1.68	0.58
2:G:119:TRP:CD1	2:G:120:ASN:N	2.71	0.58
1:B:56:ALA:HB1	1:B:63:LYS:HA	1.84	0.58
2:C:55:SER:OG	2:C:69:PRO:HG3	2.03	0.58
1:B:116:VAL:HG12	1:B:118:ASN:H	1.69	0.58
1:E:61:MET:HE3	1:E:66:TYR:HD1	1.68	0.58
1:A:95:PHE:HD1	1:A:111:PHE:HE1	1.52	0.58
1:B:106:PHE:HA	2:C:65:LEU:HD23	1.85	0.58
1:A:59:MET:HG3	1:A:66:TYR:HE1	1.68	0.58
2:H:182:GLU:CG	2:H:183:PRO:HD2	2.29	0.58
1:B:20:LEU:CD1	1:B:36:LEU:HB2	2.34	0.58
2:G:57:ARG:NH1	2:G:119:TRP:CH2	2.72	0.58
1:A:37:THR:HG23	1:A:41:SER:O	2.03	0.58
1:B:63:LYS:HZ3	1:B:63:LYS:H	1.50	0.58
1:A:131:LEU:O	1:A:134:ILE:HG12	2.04	0.57
2:G:57:ARG:CB	2:G:57:ARG:NH1	2.67	0.57
2:D:41:LEU:HD11	2:D:206:ASP:HA	1.84	0.57
2:D:75:HIS:HE1	2:D:117:PHE:HD2	1.51	0.57
2:H:201:ALA:O	2:H:203:SER:N	2.34	0.57
1:A:103:ASP:HA	1:A:104:VAL:HB	1.85	0.57
2:G:94:THR:HG22	2:G:109:ARG:HB2	1.84	0.57
2:D:97:CYS:SG	2:D:104:LEU:HD11	2.44	0.57
1:A:70:LEU:HD11	1:A:97:PHE:CE1	2.39	0.57
2:D:37:LEU:CD1	2:D:46:HIS:HB2	2.31	0.57
2:C:31:LYS:O	2:C:32:GLN:CB	2.52	0.57
2:G:146:LEU:HD13	2:H:146:LEU:HB2	1.85	0.57
1:E:99:LYS:HE2	1:E:101:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:HIS:HD2	1:B:14:PRO:HA	1.69	0.57
1:E:110:SER:O	1:E:111:PHE:HD2	1.87	0.57
2:H:17:GLN:O	2:H:18:LEU:HD23	2.04	0.57
2:C:18:LEU:HB2	2:C:96:SER:HA	1.86	0.57
1:A:107:ARG:O	1:A:108:LEU:HB2	2.04	0.57
2:D:174:LEU:CG	2:D:175:ILE:H	2.12	0.57
1:E:59:MET:O	1:E:60:ALA:CB	2.53	0.57
1:B:51:GLU:HA	1:B:54:GLN:HB3	1.87	0.57
2:G:72:PHE:CE1	2:G:117:PHE:CZ	2.92	0.57
1:E:86:PHE:CD1	1:E:86:PHE:N	2.73	0.57
2:C:147:GLN:HE21	2:C:151:ARG:HD3	1.70	0.57
2:G:94:THR:HG21	2:G:109:ARG:NH1	2.16	0.57
2:C:13:TRP:CZ2	2:C:26:LYS:HE3	2.40	0.57
1:B:116:VAL:HG12	1:B:117:GLU:N	2.19	0.57
2:G:44:VAL:HB	2:G:126:ALA:HB3	1.86	0.57
1:E:104:VAL:HB	1:E:106:PHE:HE2	1.68	0.57
1:F:36:LEU:HD23	1:F:43:TRP:HE3	1.70	0.57
1:E:118:ASN:HB2	1:E:121:GLU:HB3	1.86	0.57
1:F:119:PRO:O	1:F:123:ILE:HG13	2.05	0.57
1:B:105:SER:O	1:B:106:PHE:C	2.43	0.57
2:C:33:GLY:HA3	2:C:49:VAL:O	2.05	0.57
1:A:68:GLY:O	1:A:72:LYS:CG	2.53	0.57
2:C:211:VAL:HG13	2:C:212:MET:H	1.70	0.57
1:A:101:LEU:O	1:A:102:LYS:HG3	2.05	0.56
2:H:109:ARG:HG3	2:H:118:TYR:HE2	1.70	0.56
1:B:126:LEU:HD12	1:B:127:ILE:N	2.19	0.56
2:H:206:ASP:N	2:H:206:ASP:OD1	2.32	0.56
1:A:88:PHE:HE2	1:A:90:LYS:HA	1.69	0.56
2:D:160:LYS:O	2:D:164:ILE:HG13	2.05	0.56
2:D:58:ALA:CB	2:D:72:PHE:CZ	2.83	0.56
2:G:36:LEU:HD11	2:G:38:VAL:HG23	1.87	0.56
2:G:167:TYR:CE1	2:H:174:LEU:HD13	2.41	0.56
1:B:96:PHE:CZ	2:H:-1:GLY:C	2.79	0.56
2:H:11:GLN:OE1	2:H:12:PRO:HD2	2.06	0.56
2:H:112:LEU:CD2	2:H:117:PHE:HD1	2.15	0.56
1:A:9:HIS:CE1	1:A:17:THR:OG1	2.59	0.56
2:G:129:SER:O	2:G:132:SER:HB3	2.05	0.56
1:E:49:GLU:HA	1:E:52:ILE:HD12	1.87	0.56
1:A:130:CYS:O	1:A:134:ILE:HG12	2.05	0.56
2:C:16:LEU:O	2:C:17:GLN:HB3	2.05	0.56
1:E:74:LEU:HD23	1:E:86:PHE:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:TRP:HA	2:H:124:MET:O	2.05	0.56
2:H:38:VAL:HG12	2:H:39:SER:N	2.21	0.56
2:D:107:ARG:HG2	2:D:120:ASN:HB3	1.86	0.56
2:C:92:GLU:O	2:C:93:ALA:HB2	2.06	0.56
2:D:106:LEU:HB3	2:D:121:PHE:HB2	1.86	0.56
1:B:106:PHE:CD1	2:C:115:LEU:HD12	2.36	0.56
1:E:73:ALA:HB1	1:E:97:PHE:CE2	2.41	0.56
2:H:200:GLU:CD	2:H:201:ALA:H	2.09	0.56
1:B:43:TRP:CH2	1:B:90:LYS:HE2	2.40	0.56
2:H:57:ARG:HA	2:H:60:GLU:HG3	1.88	0.56
1:A:4:LYS:C	1:A:5:ILE:HG13	2.26	0.56
2:G:83:LEU:HD13	2:G:92:GLU:HG2	1.87	0.56
2:C:119:TRP:CD1	2:C:120:ASN:N	2.74	0.55
1:A:68:GLY:O	1:A:71:ARG:HB2	2.06	0.55
2:D:152:GLU:HA	2:D:155:THR:HG22	1.88	0.55
2:H:1:MET:O	2:H:2:GLU:C	2.45	0.55
1:B:22:VAL:HG12	1:B:24:TRP:HE3	1.71	0.55
1:B:59:MET:O	2:C:116:PRO:HG3	2.05	0.55
2:C:112:LEU:HD12	2:C:113:SER:H	1.71	0.55
2:H:142:MET:HG2	2:H:217:LEU:HG	1.87	0.55
2:H:-1:GLY:C	2:H:1:MET:H	2.09	0.55
1:A:122:VAL:O	1:A:125:GLU:N	2.40	0.55
2:H:184:PHE:C	2:H:184:PHE:CD1	2.80	0.55
1:B:104:VAL:HG12	2:C:67:ALA:HA	1.88	0.55
1:B:107:ARG:NH1	2:C:64:ARG:CG	2.69	0.55
1:F:24:TRP:HZ3	1:F:75:LEU:HD21	1.72	0.55
1:A:37:THR:HG22	1:A:39:GLY:N	2.20	0.55
2:C:146:LEU:HB2	2:D:146:LEU:HD13	1.89	0.55
2:D:171:GLY:O	2:D:172:ALA:CB	2.54	0.55
1:B:27:THR:HG22	1:B:29:GLU:H	1.71	0.55
2:C:5:GLU:HG3	2:C:48:GLN:NE2	2.21	0.55
2:H:96:SER:O	2:H:106:LEU:CD1	2.54	0.55
2:C:16:LEU:HD12	2:C:18:LEU:HD12	1.89	0.55
2:C:175:ILE:HG12	2:D:167:TYR:CZ	2.41	0.55
1:B:24:TRP:CZ3	1:B:75:LEU:HD21	2.41	0.55
1:E:19:PHE:HE1	1:F:131:LEU:HD12	1.71	0.55
1:A:7:ARG:NH2	1:B:131:LEU:HD13	2.22	0.55
1:E:84:TYR:CD2	1:E:84:TYR:N	2.74	0.54
2:C:3:GLU:O	2:C:6:GLN:HB2	2.07	0.54
2:H:7:GLY:HA2	2:H:10:MET:HG2	1.88	0.54
2:D:218:TYR:CD2	2:D:218:TYR:C	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:THR:HG22	1:E:39:GLY:N	2.21	0.54
2:C:198:LEU:N	2:C:199:PRO:CD	2.69	0.54
1:B:101:LEU:O	1:B:106:PHE:HZ	1.90	0.54
2:C:112:LEU:HD12	2:C:113:SER:N	2.22	0.54
1:E:133:THR:HG21	1:F:134:ILE:HD13	1.87	0.54
2:G:93:ALA:HB3	2:G:110:SER:HB3	1.87	0.54
2:C:167:TYR:CE2	2:D:164:ILE:HG22	2.42	0.54
2:C:29:ILE:HD13	2:C:34:TYR:HB2	1.90	0.54
1:F:99:LYS:HD3	1:F:101:LEU:HD12	1.89	0.54
1:A:53:SER:OG	1:A:63:LYS:HD3	2.07	0.54
1:B:106:PHE:HA	2:C:65:LEU:CD2	2.37	0.54
2:H:81:ARG:O	2:H:82:PRO:C	2.45	0.54
1:A:83:VAL:O	1:A:100:ASN:HB3	2.08	0.54
1:A:43:TRP:CH2	1:A:90:LYS:HE2	2.43	0.54
2:G:25:ALA:HA	2:G:37:LEU:O	2.07	0.54
2:H:7:GLY:C	2:H:9:LEU:N	2.61	0.54
2:G:175:ILE:HG22	2:G:176:ARG:H	1.72	0.54
1:A:4:LYS:CG	1:A:5:ILE:N	2.71	0.54
2:C:38:VAL:HG12	2:C:39:SER:H	1.72	0.54
1:E:19:PHE:HZ	1:F:128:CYS:SG	2.31	0.54
1:B:107:ARG:CG	2:C:64:ARG:HB3	2.37	0.54
2:H:139:LEU:O	2:H:142:MET:HB2	2.08	0.54
2:G:59:LYS:O	2:G:60:GLU:C	2.46	0.54
1:A:35:THR:HG23	1:A:43:TRP:O	2.07	0.54
2:D:67:ALA:HB1	2:D:68:PRO:HD2	1.89	0.54
2:H:92:GLU:O	2:H:93:ALA:HB3	2.03	0.54
1:A:138:GLN:O	1:A:138:GLN:HG2	2.07	0.54
1:B:42:ALA:HB3	1:B:119:PRO:HA	1.90	0.54
2:G:146:LEU:O	2:G:150:VAL:HG23	2.08	0.54
1:A:43:TRP:CZ2	1:A:90:LYS:HG2	2.43	0.53
2:C:34:TYR:C	2:C:34:TYR:HD1	2.11	0.53
2:H:146:LEU:O	2:H:150:VAL:HG23	2.08	0.53
2:H:148:CYS:O	2:H:151:ARG:HB2	2.08	0.53
1:E:107:ARG:HG3	1:E:108:LEU:H	1.73	0.53
2:G:61:LEU:HD12	2:G:62:ASN:OD1	2.08	0.53
2:C:145:ALA:HA	2:D:201:ALA:HB1	1.90	0.53
2:C:204:ILE:HD12	2:D:140:MET:SD	2.48	0.53
2:G:119:TRP:CD1	2:G:119:TRP:C	2.80	0.53
2:H:175:ILE:HG22	2:H:176:ARG:N	2.22	0.53
2:H:23:LEU:O	2:H:24:LEU:HD23	2.08	0.53
2:D:71:ALA:O	2:D:74:CYS:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:HD2	1:A:129:TYR:CE1	2.43	0.53
2:D:182:GLU:CG	2:D:183:PRO:HD2	2.38	0.53
2:H:32:GLN:O	2:H:51:THR:HG23	2.08	0.53
2:C:119:TRP:HE1	2:C:121:PHE:HD1	1.57	0.53
1:B:133:THR:C	1:B:135:ALA:N	2.62	0.53
2:C:135:LEU:O	2:C:139:LEU:HD13	2.08	0.53
2:D:15:TRP:O	2:D:16:LEU:HD12	2.08	0.53
1:E:118:ASN:ND2	1:E:121:GLU:OE1	2.41	0.53
2:D:96:SER:O	2:D:106:LEU:HD12	2.09	0.53
1:E:130:CYS:SG	1:F:130:CYS:HB3	2.48	0.53
2:C:112:LEU:HD11	2:C:115:LEU:HB2	1.89	0.53
1:A:59:MET:O	1:A:60:ALA:CB	2.56	0.53
2:G:163:GLU:OE2	2:H:164:ILE:HG21	2.07	0.53
2:C:122:HIS:CD2	2:G:101:ALA:HA	2.44	0.53
1:A:128:CYS:SG	1:B:19:PHE:HZ	2.32	0.53
1:A:130:CYS:O	1:A:134:ILE:HG23	2.08	0.53
1:A:35:THR:HG23	1:A:44:THR:OG1	2.07	0.53
2:D:215:GLN:O	2:D:218:TYR:HB3	2.08	0.53
2:D:114:GLY:O	2:D:115:LEU:HD23	2.09	0.53
1:A:45:GLY:N	1:A:113:LEU:HD22	2.24	0.53
2:D:218:TYR:HE2	2:D:222:THR:HG1	1.52	0.53
1:E:34:ILE:HG21	1:E:111:PHE:CE1	2.43	0.53
1:F:86:PHE:HB3	1:F:95:PHE:HZ	1.72	0.53
2:H:62:ASN:HB3	2:H:65:LEU:CD2	2.39	0.53
1:A:61:MET:CB	1:A:65:LYS:HD3	2.27	0.53
1:A:116:VAL:HG12	1:A:117:GLU:H	1.74	0.53
1:B:84:TYR:HD1	1:B:97:PHE:CZ	2.25	0.53
1:B:22:VAL:HG12	1:B:24:TRP:CE3	2.44	0.52
2:D:217:LEU:O	2:D:220:ALA:HB3	2.08	0.52
2:C:144:LEU:N	2:D:214:LEU:HD11	2.24	0.52
2:H:100:VAL:O	2:H:101:ALA:C	2.48	0.52
2:H:4:LEU:HD23	2:H:35:ALA:HB2	1.91	0.52
2:C:106:LEU:HD12	2:C:107:ARG:H	1.73	0.52
2:G:111:GLU:HG2	2:G:114:GLY:O	2.09	0.52
1:B:44:THR:O	1:B:114:GLU:HG2	2.09	0.52
2:G:119:TRP:NE1	2:G:121:PHE:CD1	2.77	0.52
2:G:57:ARG:CG	2:G:57:ARG:NH1	2.66	0.52
1:A:49:GLU:O	1:A:52:ILE:HG12	2.08	0.52
1:B:100:ASN:O	1:B:101:LEU:HB2	2.10	0.52
1:A:101:LEU:O	1:A:102:LYS:CB	2.57	0.52
1:A:134:ILE:CG2	1:B:134:ILE:HG12	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:9:LEU:O	2:H:11:GLN:O	2.27	0.52
2:H:211:VAL:O	2:H:215:GLN:HG2	2.09	0.52
1:B:24:TRP:HZ3	1:B:75:LEU:HD21	1.74	0.52
1:B:118:ASN:HB3	1:B:121:GLU:CB	2.38	0.52
1:A:3:ARG:HD2	1:A:129:TYR:CZ	2.44	0.52
1:F:104:VAL:CG1	2:G:67:ALA:HB2	2.40	0.52
1:B:88:PHE:HD1	1:B:95:PHE:HB2	1.75	0.52
2:C:18:LEU:HB2	2:C:96:SER:CA	2.40	0.52
2:C:179:LEU:HD23	2:D:162:LEU:HB3	1.92	0.52
1:B:64:GLY:O	1:B:67:VAL:N	2.43	0.52
2:C:34:TYR:C	2:C:34:TYR:CD1	2.83	0.52
2:H:54:VAL:O	2:H:58:ALA:HB3	2.09	0.52
2:D:61:LEU:HD11	2:D:120:ASN:OD1	2.10	0.52
1:E:51:GLU:HA	1:E:54:GLN:HB3	1.90	0.52
2:C:17:GLN:C	2:C:18:LEU:HD13	2.30	0.52
2:G:72:PHE:HE1	2:G:117:PHE:CZ	2.28	0.52
2:G:164:ILE:HG23	2:H:164:ILE:CG1	2.27	0.52
2:C:170:SER:HB3	2:D:175:ILE:CD1	2.40	0.52
2:G:192:GLN:HG3	2:G:193:PHE:N	2.25	0.52
2:D:194:MET:HA	2:D:198:LEU:HB2	1.91	0.52
1:B:101:LEU:O	1:B:106:PHE:CZ	2.63	0.51
2:G:119:TRP:NE1	2:G:121:PHE:N	2.58	0.51
1:A:25:GLU:HG3	1:A:26:LYS:N	2.24	0.51
2:C:150:VAL:HG13	2:D:153:LEU:HD11	1.91	0.51
1:F:29:GLU:HA	1:F:52:ILE:HD13	1.91	0.51
2:C:107:ARG:HD3	2:C:109:ARG:HH12	1.76	0.51
2:G:63:LYS:HG3	2:G:64:ARG:H	1.75	0.51
1:A:92:SER:C	1:A:94:TYR:H	2.13	0.51
2:G:16:LEU:HD12	2:G:18:LEU:HD12	1.91	0.51
2:C:199:PRO:HA	2:D:224:GLN:OE1	2.10	0.51
2:D:40:ASP:O	2:D:41:LEU:HB2	2.09	0.51
1:B:109:GLY:O	1:B:110:SER:HB3	2.11	0.51
2:C:148:CYS:HB3	2:D:193:PHE:HZ	1.75	0.51
1:E:110:SER:C	1:E:111:PHE:CD2	2.84	0.51
2:H:12:PRO:HD3	2:H:219:MET:SD	2.50	0.51
1:A:99:LYS:HE3	1:A:101:LEU:HD13	1.90	0.51
1:F:49:GLU:HA	1:F:52:ILE:HD12	1.92	0.51
1:B:69:GLU:OE1	1:B:99:LYS:HD2	2.10	0.51
1:B:89:SER:HB3	1:B:92:SER:HB2	1.92	0.51
1:E:106:PHE:CD2	1:E:106:PHE:N	2.78	0.51
2:G:190:LEU:O	2:G:194:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:ILE:O	2:D:168:GLN:HG3	2.10	0.51
2:D:101:ALA:C	2:D:103:ALA:H	2.14	0.51
2:C:104:LEU:HD23	2:C:105:ILE:N	2.26	0.51
1:F:37:THR:HG23	1:F:38:ASP:N	2.26	0.51
1:F:126:LEU:C	1:F:126:LEU:HD23	2.31	0.51
1:B:104:VAL:HG13	2:C:68:PRO:HD2	1.93	0.51
2:H:2:GLU:C	2:H:4:LEU:N	2.63	0.51
1:F:107:ARG:HG2	1:F:108:LEU:N	2.10	0.51
1:A:88:PHE:CD2	1:A:89:SER:N	2.79	0.51
2:C:100:VAL:HG12	2:G:105:ILE:HD12	1.92	0.51
2:G:146:LEU:HB2	2:H:146:LEU:HD13	1.92	0.51
2:G:63:LYS:O	2:G:64:ARG:C	2.50	0.51
2:D:218:TYR:C	2:D:218:TYR:HD2	2.14	0.51
2:D:198:LEU:N	2:D:199:PRO:CD	2.73	0.51
1:A:43:TRP:CZ2	1:A:90:LYS:HD3	2.46	0.51
2:D:176:ARG:O	2:D:178:ARG:N	2.43	0.51
2:C:135:LEU:HB3	2:C:136:ILE:CD1	2.33	0.51
2:H:197:LYS:C	2:H:199:PRO:HD2	2.31	0.51
1:B:94:TYR:HA	1:B:112:ASN:HA	1.92	0.51
2:H:109:ARG:HA	2:H:117:PHE:O	2.11	0.50
2:G:51:THR:HA	2:G:54:VAL:HG22	1.93	0.50
1:A:86:PHE:N	1:A:86:PHE:CD1	2.79	0.50
1:A:11:VAL:O	1:A:14:PRO:HD3	2.11	0.50
2:C:83:LEU:C	2:C:83:LEU:HD12	2.32	0.50
2:D:13:TRP:CH2	2:D:37:LEU:HD23	2.46	0.50
2:C:13:TRP:CE3	2:C:24:LEU:HD13	2.46	0.50
1:A:3:ARG:HG3	1:A:129:TYR:CZ	2.47	0.50
2:G:40:ASP:O	2:G:41:LEU:HB2	2.11	0.50
2:H:188:SER:HA	2:H:191:GLU:HG2	1.93	0.50
1:B:107:ARG:NH2	2:H:0:SER:CB	2.75	0.50
1:B:82:ASP:HB3	1:B:99:LYS:NZ	2.26	0.50
2:H:219:MET:HA	2:H:222:THR:OG1	2.11	0.50
1:A:115:LYS:C	1:A:116:VAL:O	2.48	0.50
1:F:36:LEU:HD23	1:F:43:TRP:CE3	2.46	0.50
1:E:3:ARG:HD2	1:E:129:TYR:CE2	2.47	0.50
2:G:175:ILE:HG12	2:H:167:TYR:OH	2.10	0.50
2:D:53:VAL:HG11	2:D:57:ARG:NH2	2.27	0.50
1:E:8:ILE:HD12	1:E:86:PHE:HB2	1.93	0.50
2:C:49:VAL:HG22	2:C:53:VAL:HG11	1.93	0.50
2:D:57:ARG:CZ	2:D:122:HIS:HD2	2.25	0.50
1:E:11:VAL:HB	1:E:87:ASN:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:LYS:O	2:H:64:ARG:C	2.50	0.50
1:E:10:LEU:HG	1:E:18:HIS:CG	2.46	0.50
2:H:18:LEU:CD1	2:H:97:CYS:HB3	2.42	0.50
1:A:118:ASN:O	1:A:120:ALA:N	2.44	0.50
2:D:211:VAL:CA	2:D:215:GLN:HB2	2.40	0.50
1:B:102:LYS:O	1:B:103:ASP:O	2.30	0.50
1:A:82:ASP:HB3	1:A:84:TYR:HE2	1.71	0.50
2:D:18:LEU:HB2	2:D:21:ASN:O	2.11	0.50
1:B:116:VAL:CG1	1:B:117:GLU:N	2.74	0.50
2:C:62:ASN:CB	2:C:65:LEU:HB2	2.42	0.50
2:H:4:LEU:O	2:H:5:GLU:O	2.30	0.50
1:E:3:ARG:HD3	1:E:21:GLN:OE1	2.12	0.50
1:F:89:SER:HG	1:F:91:GLU:HG2	1.76	0.50
2:D:206:ASP:OD2	2:D:208:LYS:HB3	2.12	0.50
2:D:173:THR:O	2:D:174:LEU:HB3	2.10	0.49
2:H:91:SER:O	2:H:92:GLU:O	2.30	0.49
1:B:119:PRO:O	1:B:123:ILE:HG13	2.12	0.49
2:H:25:ALA:HA	2:H:37:LEU:O	2.11	0.49
1:B:107:ARG:O	1:B:108:LEU:CB	2.58	0.49
1:B:107:ARG:CD	1:B:108:LEU:H	2.23	0.49
2:H:3:GLU:O	2:H:4:LEU:O	2.30	0.49
1:F:106:PHE:CD1	2:G:115:LEU:HD12	2.47	0.49
2:G:178:ARG:C	2:G:179:LEU:HD12	2.32	0.49
2:D:69:PRO:O	2:D:70:ALA:C	2.49	0.49
1:F:88:PHE:CE2	1:F:90:LYS:HA	2.46	0.49
2:D:175:ILE:CG2	2:D:176:ARG:N	2.74	0.49
2:D:135:LEU:O	2:D:139:LEU:HD12	2.11	0.49
1:B:8:ILE:HG13	1:B:9:HIS:N	2.25	0.49
2:G:134:HIS:O	2:G:138:PRO:HG2	2.11	0.49
2:C:38:VAL:HG12	2:C:39:SER:N	2.27	0.49
1:A:133:THR:HG22	1:B:134:ILE:HD13	1.94	0.49
1:B:104:VAL:CG1	2:C:67:ALA:CA	2.84	0.49
2:G:45:TRP:HB3	2:G:123:CYS:HB3	1.94	0.49
1:E:106:PHE:N	1:E:106:PHE:HD2	2.11	0.49
2:C:42:GLN:HA	2:D:132:SER:CB	2.43	0.49
2:D:117:PHE:CD1	2:D:118:TYR:N	2.81	0.49
1:B:4:LYS:HG3	1:B:5:ILE:N	2.26	0.49
2:C:130:LEU:HD22	2:C:134:HIS:CD2	2.48	0.49
2:H:5:GLU:OE2	2:H:134:HIS:HE1	1.95	0.49
2:H:64:ARG:HH12	2:H:116:PRO:CG	2.25	0.49
1:A:8:ILE:HD13	1:A:20:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:THR:HG21	2:D:159:MET:HB3	1.94	0.49
2:C:217:LEU:HA	2:C:220:ALA:HB3	1.95	0.49
1:E:131:LEU:CD1	1:F:19:PHE:HE1	2.26	0.49
1:B:10:LEU:HD12	1:B:18:HIS:CG	2.47	0.49
2:C:105:ILE:HG13	2:G:101:ALA:H	1.77	0.49
2:G:157:LEU:HD13	2:G:184:PHE:CE1	2.48	0.49
2:H:103:ALA:CA	2:H:123:CYS:O	2.61	0.49
1:A:13:GLU:C	1:A:15:SER:H	2.16	0.49
1:E:45:GLY:HA3	1:E:113:LEU:HD23	1.95	0.49
2:G:198:LEU:HD21	2:H:220:ALA:HB1	1.95	0.49
2:C:37:LEU:HD12	2:C:45:TRP:O	2.12	0.49
2:G:57:ARG:CB	2:G:57:ARG:HH11	2.24	0.49
2:H:15:TRP:HA	2:H:24:LEU:HD22	1.95	0.49
1:E:7:ARG:HH21	1:F:131:LEU:HD13	1.77	0.49
1:E:95:PHE:CE2	1:E:97:PHE:HB3	2.48	0.48
1:F:6:SER:HB3	1:F:76:SER:HB2	1.95	0.48
2:C:206:ASP:N	2:C:206:ASP:OD1	2.45	0.48
1:A:2:GLU:O	1:A:3:ARG:HB3	2.13	0.48
1:A:111:PHE:CD1	1:A:111:PHE:N	2.77	0.48
2:C:105:ILE:HG13	2:G:101:ALA:N	2.28	0.48
2:G:36:LEU:HG	2:G:37:LEU:N	2.26	0.48
1:A:52:ILE:HG13	1:A:53:SER:N	2.27	0.48
2:C:202:CYS:HB2	2:D:141:GLY:CA	2.42	0.48
2:H:5:GLU:HG3	2:H:6:GLN:N	2.28	0.48
1:A:84:TYR:HE1	1:A:99:LYS:HD3	1.78	0.48
2:C:179:LEU:HD13	2:D:166:ASP:OD2	2.12	0.48
2:C:16:LEU:CD2	2:C:83:LEU:HD21	2.33	0.48
1:A:118:ASN:CB	1:A:121:GLU:HG2	2.32	0.48
2:G:17:GLN:C	2:G:18:LEU:HD13	2.34	0.48
2:C:31:LYS:HA	2:C:73:LEU:HD11	1.95	0.48
2:G:136:ILE:O	2:G:139:LEU:N	2.46	0.48
2:G:49:VAL:HG21	2:G:53:VAL:HG11	1.96	0.48
1:A:25:GLU:HG3	1:A:26:LYS:H	1.78	0.48
1:A:72:LYS:HB3	1:A:77:GLY:O	2.13	0.48
2:H:119:TRP:NE1	2:H:121:PHE:HA	2.23	0.48
2:G:63:LYS:NZ	2:G:63:LYS:HB2	2.28	0.48
2:D:62:ASN:ND2	2:D:117:PHE:HE1	2.09	0.48
1:A:10:LEU:N	1:A:10:LEU:HD23	2.28	0.48
2:D:152:GLU:O	2:D:156:LEU:HD12	2.13	0.48
2:C:25:ALA:HB2	2:C:38:VAL:HA	1.94	0.48
1:B:64:GLY:O	1:B:67:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:185:GLU:HB3	2:G:188:SER:OG	2.14	0.48
1:B:99:LYS:HB3	1:B:107:ARG:O	2.14	0.48
1:B:96:PHE:HE1	1:B:98:GLU:OE1	1.96	0.48
2:D:132:SER:HA	2:D:136:ILE:HD12	1.95	0.48
2:H:202:CYS:O	2:H:202:CYS:SG	2.71	0.48
2:C:218:TYR:CD2	2:C:218:TYR:C	2.86	0.48
2:C:107:ARG:HB3	2:C:109:ARG:NH1	2.27	0.48
2:G:55:SER:OG	2:G:69:PRO:HG3	2.14	0.48
1:E:96:PHE:CD1	1:E:96:PHE:O	2.63	0.48
1:F:72:LYS:O	1:F:78:ALA:HB2	2.13	0.48
2:D:107:ARG:HG2	2:D:120:ASN:HB2	1.96	0.48
2:H:217:LEU:O	2:H:221:VAL:HG23	2.14	0.48
1:F:3:ARG:HD3	1:F:21:GLN:OE1	2.13	0.48
1:B:113:LEU:HB3	1:B:114:GLU:H	1.53	0.48
2:G:189:PHE:CE2	2:H:149:GLN:HG3	2.48	0.48
2:D:8:LEU:HD22	2:D:35:ALA:HB1	1.96	0.48
2:C:119:TRP:NE1	2:C:121:PHE:CD1	2.82	0.48
1:A:101:LEU:O	1:A:102:LYS:HB2	2.13	0.48
1:A:84:TYR:CE1	1:A:99:LYS:HD3	2.48	0.48
1:F:97:PHE:CE1	1:F:109:GLY:HA3	2.49	0.48
2:G:8:LEU:O	2:G:26:LYS:HD3	2.13	0.48
1:F:99:LYS:HG2	1:F:100:ASN:H	1.78	0.48
1:E:118:ASN:N	1:E:118:ASN:OD1	2.46	0.48
2:H:8:LEU:HD13	2:H:26:LYS:HG3	1.96	0.48
2:H:5:GLU:O	2:H:8:LEU:CB	2.55	0.48
1:E:107:ARG:O	1:E:108:LEU:CB	2.54	0.48
2:C:124:MET:O	2:C:125:LEU:C	2.52	0.48
1:F:106:PHE:CD2	1:F:106:PHE:N	2.80	0.48
2:D:98:ASP:O	2:D:104:LEU:HD12	2.14	0.48
1:B:27:THR:O	1:B:29:GLU:N	2.47	0.48
2:C:176:ARG:NH2	2:C:179:LEU:HD11	2.29	0.48
2:G:189:PHE:HE2	2:H:149:GLN:HG3	1.79	0.48
2:C:193:PHE:CE2	2:D:149:GLN:HG3	2.49	0.48
1:A:119:PRO:CG	1:A:120:ALA:H	2.25	0.47
2:C:169:GLU:CG	2:C:170:SER:N	2.77	0.47
2:C:105:ILE:HG22	2:C:105:ILE:O	2.14	0.47
2:D:18:LEU:CD2	2:D:95:PHE:HB3	2.44	0.47
1:A:49:GLU:O	1:A:52:ILE:CG1	2.62	0.47
1:A:73:ALA:HB2	1:A:84:TYR:CE1	2.48	0.47
2:G:108:VAL:HG23	2:G:108:VAL:O	2.14	0.47
2:H:131:VAL:O	2:H:136:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:NH2	1:B:131:LEU:HB3	2.29	0.47
1:E:134:ILE:HG13	1:E:135:ALA:N	2.29	0.47
2:G:54:VAL:CG2	2:G:69:PRO:HB3	2.42	0.47
1:A:40:HIS:O	1:A:119:PRO:HB2	2.13	0.47
1:B:37:THR:CG2	1:B:39:GLY:H	2.27	0.47
1:A:99:LYS:CB	1:A:108:LEU:HD12	2.44	0.47
1:A:118:ASN:HD22	1:A:121:GLU:CD	2.17	0.47
2:H:131:VAL:HG13	2:H:135:LEU:HD23	1.96	0.47
1:A:8:ILE:HD13	1:A:20:LEU:HD11	1.96	0.47
1:A:131:LEU:HD13	1:B:7:ARG:HD3	1.97	0.47
2:H:1:MET:O	2:H:3:GLU:HB3	2.15	0.47
2:H:5:GLU:CG	2:H:6:GLN:N	2.75	0.47
2:D:174:LEU:HD23	2:D:177:ASP:HA	1.95	0.47
1:A:27:THR:HG22	1:A:28:LEU:N	2.29	0.47
2:G:140:MET:CE	2:H:207:GLY:HA2	2.45	0.47
1:B:83:VAL:O	1:B:100:ASN:O	2.33	0.47
2:G:60:GLU:O	2:G:61:LEU:CB	2.62	0.47
2:C:166:ASP:OD2	2:D:179:LEU:HD11	2.14	0.47
2:G:142:MET:HE3	2:G:217:LEU:HD23	1.96	0.47
1:B:109:GLY:O	1:B:110:SER:CB	2.60	0.47
2:H:106:LEU:HB3	2:H:121:PHE:HB2	1.96	0.47
1:A:107:ARG:O	1:A:108:LEU:CB	2.63	0.47
2:G:58:ALA:HB1	2:G:72:PHE:CZ	2.49	0.47
1:F:97:PHE:CE2	1:F:108:LEU:HB3	2.50	0.47
1:F:3:ARG:HG2	1:F:4:LYS:N	2.29	0.47
1:B:86:PHE:O	1:B:87:ASN:ND2	2.48	0.47
2:G:170:SER:HB3	2:H:175:ILE:CD1	2.43	0.47
2:G:167:TYR:HE1	2:H:174:LEU:HD13	1.78	0.47
1:F:116:VAL:HG12	1:F:118:ASN:H	1.79	0.47
2:G:49:VAL:CG1	2:G:50:ASP:N	2.77	0.47
2:D:217:LEU:O	2:D:221:VAL:HG23	2.15	0.47
2:C:191:GLU:HG3	2:C:192:GLN:N	2.30	0.47
2:C:204:ILE:O	2:C:209:PRO:HD2	2.14	0.47
2:D:131:VAL:O	2:D:136:ILE:HG13	2.15	0.47
1:B:10:LEU:HD12	1:B:18:HIS:CD2	2.50	0.47
1:B:88:PHE:HE2	1:B:90:LYS:HA	1.80	0.47
2:H:149:GLN:O	2:H:153:LEU:HG	2.15	0.47
1:F:53:SER:HA	1:F:63:LYS:HD3	1.97	0.47
1:B:83:VAL:O	1:B:100:ASN:HB3	2.14	0.47
2:H:-1:GLY:H3	2:H:32:GLN:HE21	1.60	0.47
1:A:117:GLU:O	1:A:119:PRO:CD	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:TYR:CE2	2:D:222:THR:OG1	2.66	0.47
1:B:73:ALA:HB2	1:B:84:TYR:CE1	2.50	0.47
2:D:65:LEU:H	2:D:65:LEU:HD22	1.80	0.47
2:H:218:TYR:CE2	2:H:222:THR:HG21	2.50	0.46
1:E:86:PHE:N	1:E:86:PHE:HD1	2.13	0.46
2:G:95:PHE:HD2	2:G:108:VAL:HG12	1.80	0.46
2:G:16:LEU:HD12	2:G:18:LEU:CD1	2.44	0.46
1:B:43:TRP:HD1	1:B:114:GLU:O	1.98	0.46
2:G:98:ASP:HB2	2:G:105:ILE:HG22	1.97	0.46
2:G:95:PHE:CD2	2:G:108:VAL:HG12	2.50	0.46
2:C:29:ILE:CG2	2:C:73:LEU:HB2	2.45	0.46
2:C:211:VAL:HA	2:C:215:GLN:HE21	1.80	0.46
2:D:66:THR:HG22	2:D:66:THR:O	2.14	0.46
1:A:134:ILE:HG13	1:A:135:ALA:N	2.31	0.46
2:D:211:VAL:C	2:D:215:GLN:HB2	2.35	0.46
1:E:131:LEU:HD12	1:F:19:PHE:HE1	1.80	0.46
2:G:36:LEU:HD11	2:G:38:VAL:CG2	2.44	0.46
2:C:29:ILE:HD13	2:C:34:TYR:CB	2.45	0.46
2:G:140:MET:HE1	2:H:207:GLY:HA2	1.96	0.46
1:A:88:PHE:HE1	1:A:113:LEU:HB2	1.80	0.46
2:C:145:ALA:O	2:C:148:CYS:HB2	2.14	0.46
1:F:19:PHE:O	1:F:20:LEU:HD12	2.15	0.46
2:C:131:VAL:O	2:C:136:ILE:HD13	2.15	0.46
1:B:5:ILE:HG23	1:B:20:LEU:O	2.16	0.46
1:F:100:ASN:O	1:F:101:LEU:HG	2.16	0.46
1:A:67:VAL:HG12	1:A:68:GLY:N	2.30	0.46
2:G:206:ASP:OD2	2:G:208:LYS:HB2	2.15	0.46
2:H:77:ASP:OD1	2:H:77:ASP:C	2.54	0.46
1:F:136:GLU:HG2	1:F:136:GLU:O	2.14	0.46
1:B:82:ASP:HB3	1:B:99:LYS:HZ1	1.81	0.46
2:C:136:ILE:O	2:C:137:ARG:C	2.53	0.46
2:G:18:LEU:HD22	2:G:21:ASN:O	2.15	0.46
2:G:167:TYR:HB3	2:H:167:TYR:CD2	2.50	0.46
2:C:144:LEU:HD21	2:D:210:PHE:HA	1.96	0.46
2:H:7:GLY:O	2:H:10:MET:HG2	2.16	0.46
2:G:93:ALA:HB2	2:G:110:SER:HB3	1.95	0.46
2:G:33:GLY:HA2	2:G:73:LEU:HD13	1.97	0.46
2:C:79:LEU:HD21	2:C:93:ALA:CB	2.36	0.46
2:C:32:GLN:HA	2:C:51:THR:HG23	1.97	0.46
1:A:37:THR:CG2	1:A:38:ASP:N	2.79	0.46
1:F:59:MET:O	1:F:60:ALA:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:43:GLN:HB3	2:H:128:PRO:CB	2.46	0.46
2:G:14:ALA:O	2:G:24:LEU:HD22	2.16	0.46
1:B:82:ASP:HA	1:B:101:LEU:HD22	1.97	0.46
2:C:42:GLN:HG3	2:D:132:SER:OG	2.15	0.46
2:D:62:ASN:HB3	2:D:65:LEU:CD2	2.41	0.46
1:A:28:LEU:HD11	1:A:32:PHE:CE2	2.51	0.46
2:H:65:LEU:N	2:H:65:LEU:HD22	2.27	0.46
2:C:177:ASP:OD1	2:C:180:LYS:HD2	2.16	0.46
1:B:94:TYR:CE1	1:B:112:ASN:ND2	2.84	0.46
1:B:97:PHE:CD2	1:B:108:LEU:HB3	2.50	0.46
2:H:34:TYR:HH	2:H:119:TRP:HZ2	1.64	0.46
2:D:83:LEU:HA	2:D:84:LEU:HA	1.60	0.46
2:G:152:GLU:O	2:G:156:LEU:HD12	2.16	0.46
2:G:110:SER:O	2:G:117:PHE:O	2.34	0.46
1:A:89:SER:O	1:A:92:SER:HB3	2.15	0.46
1:F:88:PHE:HE2	1:F:90:LYS:HA	1.79	0.46
2:D:5:GLU:OE2	2:D:8:LEU:HD23	2.16	0.46
2:C:188:SER:HA	2:C:191:GLU:HG2	1.98	0.46
2:C:152:GLU:O	2:C:155:THR:HG22	2.16	0.46
2:H:119:TRP:NE1	2:H:121:PHE:CA	2.78	0.45
2:C:16:LEU:HA	2:C:16:LEU:HD22	1.82	0.45
2:C:147:GLN:HB2	2:D:214:LEU:HD21	1.98	0.45
1:F:5:ILE:HG22	1:F:6:SER:N	2.31	0.45
1:B:5:ILE:CG2	1:B:6:SER:H	2.27	0.45
2:G:118:TYR:O	2:G:118:TYR:HD2	1.99	0.45
1:F:118:ASN:ND2	1:F:121:GLU:H	2.11	0.45
1:B:104:VAL:O	1:B:105:SER:HB2	2.16	0.45
2:H:6:GLN:O	2:H:8:LEU:N	2.49	0.45
2:C:18:LEU:C	2:C:20:GLU:N	2.70	0.45
2:G:119:TRP:HE1	2:G:121:PHE:N	2.14	0.45
2:G:187:ASN:O	2:G:191:GLU:HG2	2.16	0.45
2:G:198:LEU:N	2:G:199:PRO:CD	2.78	0.45
1:A:88:PHE:CZ	1:A:93:CYS:HA	2.51	0.45
2:C:144:LEU:HA	2:D:214:LEU:HD11	1.99	0.45
1:E:84:TYR:HD2	1:E:84:TYR:H	1.61	0.45
1:B:133:THR:O	1:B:136:GLU:N	2.49	0.45
1:A:5:ILE:HA	1:A:20:LEU:O	2.16	0.45
1:A:49:GLU:HA	1:A:52:ILE:HG12	1.98	0.45
2:H:80:LEU:HG	2:H:81:ARG:H	1.81	0.45
1:E:97:PHE:CE1	1:E:109:GLY:HA3	2.50	0.45
1:F:104:VAL:HG12	2:G:67:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:GLU:HA	1:F:107:ARG:CA	2.38	0.45
2:D:210:PHE:CD2	2:D:214:LEU:HB3	2.51	0.45
2:D:81:ARG:O	2:D:83:LEU:N	2.50	0.45
2:C:112:LEU:CG	2:C:113:SER:H	2.29	0.45
1:A:125:GLU:OE2	1:A:125:GLU:O	2.35	0.45
2:C:127:SER:O	2:C:131:VAL:HG23	2.17	0.45
1:F:37:THR:OG1	1:F:42:ALA:CA	2.65	0.45
1:A:126:LEU:C	1:A:126:LEU:HD23	2.37	0.45
2:C:217:LEU:HD12	2:C:220:ALA:HB3	1.99	0.45
1:E:92:SER:O	1:E:93:CYS:HB2	2.17	0.45
2:G:149:GLN:HE22	2:H:190:LEU:CD2	2.29	0.45
1:B:101:LEU:O	1:B:102:LYS:CB	2.64	0.45
2:G:119:TRP:CD1	2:G:121:PHE:N	2.85	0.45
2:G:96:SER:OG	2:G:107:ARG:HB2	2.17	0.45
2:D:80:LEU:O	2:D:81:ARG:C	2.55	0.45
2:G:153:LEU:HD11	2:H:150:VAL:HG13	1.99	0.45
1:B:31:GLY:HA2	1:B:52:ILE:HD11	1.99	0.45
2:C:185:GLU:HB3	2:C:188:SER:OG	2.16	0.45
1:A:84:TYR:CE1	1:A:99:LYS:CD	3.00	0.45
2:C:170:SER:HB3	2:D:175:ILE:CG1	2.46	0.45
2:C:41:LEU:HD13	2:C:204:ILE:HG21	1.99	0.45
2:C:129:SER:O	2:C:132:SER:HB3	2.16	0.45
1:A:59:MET:HG3	1:A:66:TYR:CE1	2.51	0.45
2:G:72:PHE:CD1	2:G:117:PHE:CZ	3.05	0.45
2:D:25:ALA:HA	2:D:37:LEU:O	2.17	0.45
2:C:42:GLN:O	2:C:43:GLN:CB	2.55	0.45
2:G:56:GLN:O	2:G:59:LYS:HB2	2.17	0.45
1:E:110:SER:C	1:E:111:PHE:HD2	2.19	0.45
1:A:29:GLU:HB2	1:A:52:ILE:CD1	2.47	0.45
1:A:70:LEU:HD11	1:A:97:PHE:CZ	2.52	0.45
1:A:70:LEU:HD11	1:A:97:PHE:HE1	1.80	0.45
2:D:64:ARG:C	2:D:65:LEU:HD13	2.37	0.44
1:A:32:PHE:HE1	1:A:47:VAL:HG21	1.74	0.44
1:A:96:PHE:HA	1:A:109:GLY:O	2.17	0.44
2:G:24:LEU:HD11	2:G:207:GLY:HA3	2.00	0.44
2:C:62:ASN:C	2:C:64:ARG:H	2.20	0.44
2:H:72:PHE:CZ	2:H:119:TRP:CZ3	3.05	0.44
2:G:51:THR:HA	2:G:54:VAL:CG2	2.47	0.44
1:A:40:HIS:O	1:A:119:PRO:CB	2.65	0.44
2:C:151:ARG:O	2:C:154:ALA:HB3	2.17	0.44
2:D:13:TRP:HD1	2:D:215:GLN:OE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:LYS:HB3	2:C:209:PRO:HD3	1.99	0.44
2:C:105:ILE:HG13	2:G:100:VAL:HG23	1.98	0.44
2:D:81:ARG:O	2:D:82:PRO:C	2.55	0.44
2:H:45:TRP:HB3	2:H:123:CYS:HB3	1.99	0.44
2:D:41:LEU:CD1	2:D:206:ASP:HA	2.47	0.44
2:H:188:SER:HA	2:H:191:GLU:CG	2.46	0.44
2:C:112:LEU:CD1	2:C:113:SER:H	2.30	0.44
2:C:62:ASN:O	2:C:64:ARG:N	2.51	0.44
1:A:66:TYR:CE1	1:A:108:LEU:CD2	2.99	0.44
1:A:32:PHE:CD1	1:A:47:VAL:HG21	2.51	0.44
1:A:61:MET:HE3	1:A:66:TYR:HD1	1.82	0.44
2:C:1:MET:O	2:C:2:GLU:C	2.56	0.44
1:A:29:GLU:C	1:A:31:GLY:H	2.21	0.44
1:E:29:GLU:HA	1:E:52:ILE:HD13	1.99	0.44
2:H:204:ILE:HG22	2:H:205:GLY:N	2.32	0.44
2:H:97:CYS:CB	2:H:106:LEU:HD13	2.47	0.44
2:H:119:TRP:CD1	2:H:121:PHE:N	2.85	0.44
2:D:68:PRO:HB2	2:D:69:PRO:HD2	2.00	0.44
2:H:6:GLN:O	2:H:9:LEU:N	2.41	0.44
2:H:72:PHE:CZ	2:H:76:LEU:HD11	2.52	0.44
2:H:97:CYS:CB	2:H:106:LEU:CD1	2.96	0.44
1:B:16:ILE:O	1:B:18:HIS:ND1	2.46	0.44
2:C:100:VAL:HG22	2:G:100:VAL:HG22	1.99	0.44
2:H:200:GLU:O	2:H:201:ALA:C	2.55	0.44
1:A:103:ASP:CA	1:A:104:VAL:HB	2.48	0.44
2:H:40:ASP:O	2:H:41:LEU:CB	2.65	0.44
2:D:38:VAL:HG12	2:D:39:SER:N	2.33	0.44
2:C:224:GLN:HE22	2:D:198:LEU:HD23	1.81	0.44
2:H:6:GLN:HB3	2:H:7:GLY:H	1.42	0.44
1:A:122:VAL:O	1:A:123:ILE:C	2.56	0.44
2:G:16:LEU:HD13	2:G:17:GLN:N	2.23	0.44
2:H:176:ARG:C	2:H:178:ARG:H	2.21	0.44
1:A:8:ILE:HD11	1:A:10:LEU:HD21	2.00	0.44
2:C:179:LEU:N	2:C:179:LEU:HD12	2.33	0.44
2:D:162:LEU:HD23	2:D:162:LEU:HA	1.78	0.44
2:D:175:ILE:CG2	2:D:176:ARG:HG2	2.39	0.44
2:G:77:ASP:O	2:G:81:ARG:HB2	2.18	0.44
1:B:125:GLU:O	1:B:128:CYS:HB2	2.17	0.44
1:F:45:GLY:HA3	1:F:113:LEU:HD23	2.00	0.44
2:H:81:ARG:O	2:H:82:PRO:O	2.36	0.44
2:H:97:CYS:C	2:H:98:ASP:OD1	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TRP:HH2	1:B:90:LYS:HE2	1.82	0.44
2:D:208:LYS:N	2:D:209:PRO:CD	2.80	0.44
1:F:29:GLU:HG3	1:F:63:LYS:HZ1	1.83	0.44
2:D:190:LEU:HD23	2:D:190:LEU:HA	1.72	0.44
1:B:94:TYR:HE2	1:B:110:SER:HB2	1.81	0.43
2:C:166:ASP:OD2	2:D:179:LEU:HD21	2.18	0.43
1:B:9:HIS:CE1	1:B:17:THR:HB	2.53	0.43
2:G:161:ASP:O	2:G:165:GLN:HB2	2.18	0.43
2:C:202:CYS:O	2:C:203:SER:C	2.56	0.43
1:E:107:ARG:CG	1:E:107:ARG:NH1	2.60	0.43
2:C:18:LEU:CD2	2:C:97:CYS:HB3	2.44	0.43
1:E:74:LEU:CD2	1:E:86:PHE:HE2	2.31	0.43
2:D:210:PHE:CE1	2:D:215:GLN:NE2	2.86	0.43
2:C:100:VAL:CG1	2:G:105:ILE:HD12	2.48	0.43
1:A:92:SER:C	1:A:94:TYR:N	2.70	0.43
2:C:136:ILE:O	2:C:139:LEU:N	2.51	0.43
2:G:136:ILE:O	2:G:137:ARG:C	2.57	0.43
2:G:34:TYR:C	2:G:34:TYR:CD1	2.92	0.43
1:B:96:PHE:CB	1:B:110:SER:HB3	2.46	0.43
2:H:80:LEU:HG	2:H:81:ARG:N	2.33	0.43
1:F:7:ARG:HB2	1:F:19:PHE:CE1	2.53	0.43
2:G:57:ARG:HB3	2:G:57:ARG:HH11	1.76	0.43
1:B:118:ASN:O	1:B:122:VAL:HG23	2.18	0.43
2:H:70:ALA:O	2:H:71:ALA:C	2.57	0.43
1:E:95:PHE:HE2	1:E:97:PHE:HB3	1.84	0.43
2:G:144:LEU:O	2:G:147:GLN:HB3	2.19	0.43
1:F:81:ALA:O	1:F:82:ASP:C	2.56	0.43
2:H:6:GLN:HE21	2:H:6:GLN:CA	2.32	0.43
1:E:99:LYS:CE	1:E:101:LEU:HD11	2.48	0.43
2:C:16:LEU:HD21	2:C:83:LEU:CD2	2.35	0.43
1:E:70:LEU:HA	1:E:73:ALA:HB3	2.00	0.43
2:D:65:LEU:N	2:D:65:LEU:CD1	2.74	0.43
1:B:8:ILE:HD11	1:B:10:LEU:HG	1.99	0.43
1:B:72:LYS:CB	1:B:78:ALA:HA	2.40	0.43
2:G:167:TYR:HD2	2:H:167:TYR:CB	2.26	0.43
1:E:82:ASP:HB2	1:E:84:TYR:CE2	2.54	0.43
2:G:189:PHE:HA	2:G:192:GLN:HG2	2.00	0.43
2:H:34:TYR:CD1	2:H:34:TYR:C	2.92	0.43
1:E:86:PHE:CD2	1:E:97:PHE:HB2	2.53	0.43
1:E:110:SER:O	1:E:111:PHE:CD2	2.69	0.43
1:E:124:ARG:CG	1:F:38:ASP:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:TRP:CZ3	1:F:75:LEU:HD21	2.53	0.43
2:D:198:LEU:N	2:D:199:PRO:HD2	2.33	0.43
2:G:58:ALA:HB1	2:G:72:PHE:CE2	2.53	0.43
2:D:109:ARG:HD2	2:D:118:TYR:HE2	1.84	0.43
1:F:73:ALA:O	1:F:86:PHE:HZ	2.02	0.43
2:C:113:SER:C	2:C:115:LEU:H	2.22	0.43
2:H:34:TYR:O	2:H:48:GLN:HA	2.19	0.43
2:H:224:GLN:HE21	2:H:224:GLN:HB2	1.48	0.43
2:H:59:LYS:HE2	2:H:66:THR:CB	2.48	0.43
2:D:110:SER:O	2:D:117:PHE:N	2.48	0.43
1:B:86:PHE:HB3	1:B:95:PHE:CE2	2.50	0.43
1:A:24:TRP:CZ3	1:A:75:LEU:HD21	2.54	0.43
2:D:39:SER:CB	2:D:44:VAL:HG22	2.48	0.43
2:C:176:ARG:HH21	2:C:179:LEU:HD11	1.84	0.43
2:G:149:GLN:HG3	2:H:193:PHE:CZ	2.54	0.43
2:C:83:LEU:O	2:C:83:LEU:HD12	2.19	0.43
2:H:112:LEU:CG	2:H:112:LEU:O	2.40	0.43
2:D:115:LEU:HD22	2:D:115:LEU:HA	1.82	0.43
2:G:159:MET:O	2:G:162:LEU:HB2	2.19	0.43
1:F:89:SER:C	1:F:91:GLU:H	2.22	0.43
2:C:117:PHE:O	2:C:118:TYR:CD2	2.72	0.43
1:E:59:MET:HE2	1:E:59:MET:HB3	1.78	0.43
1:A:47:VAL:HA	1:A:51:GLU:OE1	2.18	0.42
1:B:5:ILE:CG2	1:B:6:SER:N	2.82	0.42
1:E:19:PHE:CE1	1:F:131:LEU:HD12	2.53	0.42
1:A:126:LEU:O	1:A:129:TYR:HB3	2.19	0.42
1:E:72:LYS:HB3	1:E:84:TYR:OH	2.18	0.42
1:E:103:ASP:OD1	1:E:103:ASP:N	2.51	0.42
1:B:106:PHE:CD1	2:C:115:LEU:CD1	2.91	0.42
1:A:43:TRP:CH2	1:A:90:LYS:CE	3.02	0.42
2:C:160:LYS:HG2	2:D:181:THR:CG2	2.48	0.42
2:C:105:ILE:CG1	2:G:101:ALA:H	2.31	0.42
1:F:86:PHE:CD1	1:F:86:PHE:N	2.87	0.42
2:D:96:SER:OG	2:D:107:ARG:HB2	2.19	0.42
2:C:44:VAL:HB	2:C:126:ALA:HB3	2.01	0.42
2:H:98:ASP:N	2:H:98:ASP:OD1	2.53	0.42
2:C:160:LYS:HG2	2:D:181:THR:HG21	2.02	0.42
2:D:1:MET:HE1	2:D:50:ASP:HB3	2.00	0.42
1:B:6:SER:HB2	1:B:76:SER:HB2	2.01	0.42
1:A:7:ARG:HH22	1:B:131:LEU:HB3	1.85	0.42
1:E:28:LEU:HD22	1:E:75:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:VAL:HG12	1:B:11:VAL:O	2.20	0.42
2:H:72:PHE:CA	2:H:75:HIS:HD2	2.30	0.42
2:C:26:LYS:HD2	2:C:134:HIS:ND1	2.35	0.42
2:H:200:GLU:HG2	2:H:201:ALA:H	1.77	0.42
1:A:4:LYS:HZ3	1:A:4:LYS:HG3	1.65	0.42
1:B:49:GLU:HA	1:B:52:ILE:HD12	2.01	0.42
1:E:48:SER:O	1:E:52:ILE:HG13	2.19	0.42
2:C:142:MET:O	2:C:146:LEU:HG	2.20	0.42
2:H:47:GLU:HB2	2:H:122:HIS:O	2.20	0.42
2:G:62:ASN:ND2	2:G:117:PHE:CD1	2.72	0.42
2:G:94:THR:CG2	2:G:109:ARG:NH1	2.80	0.42
1:B:107:ARG:NH2	2:H:0:SER:OG	2.52	0.42
1:E:83:VAL:O	1:E:100:ASN:HB2	2.19	0.42
1:A:115:LYS:O	1:A:116:VAL:O	2.38	0.42
1:A:118:ASN:C	1:A:120:ALA:N	2.70	0.42
2:C:148:CYS:O	2:C:151:ARG:HB2	2.19	0.42
2:D:58:ALA:HB1	2:D:72:PHE:CE2	2.51	0.42
2:D:115:LEU:HA	2:D:116:PRO:HD2	1.70	0.42
1:B:36:LEU:HD23	1:B:43:TRP:HB2	2.01	0.42
1:B:44:THR:HG22	1:B:45:GLY:N	2.34	0.42
1:F:37:THR:OG1	1:F:42:ALA:CB	2.67	0.42
1:B:29:GLU:C	1:B:31:GLY:H	2.22	0.42
2:C:84:LEU:HD12	2:C:84:LEU:N	2.35	0.42
1:A:107:ARG:CG	1:A:108:LEU:N	2.62	0.42
2:D:117:PHE:HD1	2:D:118:TYR:H	1.68	0.42
1:B:113:LEU:O	1:B:114:GLU:HB3	2.19	0.42
1:B:62:GLU:C	1:B:64:GLY:N	2.73	0.42
1:B:84:TYR:HB3	1:B:97:PHE:HE1	1.84	0.42
2:H:36:LEU:HD22	2:H:121:PHE:CE1	2.55	0.42
2:C:96:SER:OG	2:C:107:ARG:HB2	2.18	0.42
2:G:118:TYR:CD2	2:G:119:TRP:N	2.88	0.42
1:E:87:ASN:HB2	1:E:96:PHE:CD1	2.54	0.42
2:C:153:LEU:CD1	2:D:150:VAL:HG13	2.49	0.42
2:C:181:THR:CG2	2:D:159:MET:HB3	2.50	0.42
2:H:192:GLN:O	2:H:196:GLU:HB2	2.20	0.42
2:H:29:ILE:HD13	2:H:34:TYR:HB2	2.01	0.42
2:H:79:LEU:HG	2:H:79:LEU:O	2.20	0.42
2:G:190:LEU:HA	2:G:190:LEU:HD23	1.94	0.42
2:G:179:LEU:O	2:H:163:GLU:HB2	2.20	0.42
2:C:167:TYR:CE1	2:D:174:LEU:HB2	2.55	0.42
2:C:15:TRP:CE2	2:C:206:ASP:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:ARG:O	2:H:178:ARG:N	2.53	0.42
2:C:130:LEU:C	2:C:132:SER:N	2.73	0.42
1:A:109:GLY:O	1:A:110:SER:HB3	2.19	0.42
2:G:1:MET:SD	2:G:4:LEU:HD12	2.60	0.42
2:C:66:THR:O	2:C:66:THR:OG1	2.38	0.42
1:A:43:TRP:CH2	1:A:90:LYS:HD3	2.55	0.41
1:A:96:PHE:CB	1:A:109:GLY:O	2.66	0.41
1:F:29:GLU:C	1:F:31:GLY:H	2.23	0.41
2:G:116:PRO:O	2:G:117:PHE:HB2	2.19	0.41
1:F:107:ARG:O	1:F:108:LEU:HB2	2.19	0.41
2:G:138:PRO:HB3	2:G:222:THR:HG23	2.00	0.41
1:A:68:GLY:O	1:A:72:LYS:HG2	2.20	0.41
2:H:81:ARG:HA	2:H:82:PRO:HD2	1.91	0.41
2:D:174:LEU:HD11	2:D:179:LEU:CD1	2.43	0.41
2:D:131:VAL:O	2:D:135:LEU:HB3	2.20	0.41
1:A:32:PHE:CD1	1:A:47:VAL:CG2	3.03	0.41
1:B:37:THR:HG22	1:B:39:GLY:H	1.85	0.41
1:F:37:THR:OG1	1:F:41:SER:O	2.30	0.41
1:A:13:GLU:OE1	1:A:16:ILE:HD12	2.20	0.41
2:G:15:TRP:HD1	2:G:24:LEU:HD21	1.85	0.41
2:H:-1:GLY:H1	2:H:32:GLN:NE2	2.03	0.41
2:H:78:ASN:O	2:H:79:LEU:CB	2.67	0.41
2:C:157:LEU:HD23	2:D:160:LYS:HD2	2.03	0.41
2:D:176:ARG:O	2:D:179:LEU:HG	2.20	0.41
2:G:155:THR:O	2:G:159:MET:HG2	2.20	0.41
2:C:7:GLY:O	2:C:10:MET:HB2	2.19	0.41
2:C:68:PRO:HA	2:C:69:PRO:HD3	1.96	0.41
1:E:88:PHE:CE1	1:E:113:LEU:HD12	2.55	0.41
1:B:6:SER:CB	1:B:76:SER:HB2	2.50	0.41
2:G:160:LYS:HD2	2:H:157:LEU:HD23	2.03	0.41
2:G:131:VAL:HG12	2:G:136:ILE:CD1	2.51	0.41
2:C:192:GLN:HG3	2:C:193:PHE:N	2.34	0.41
2:H:9:LEU:HD23	2:H:134:HIS:NE2	2.33	0.41
2:C:175:ILE:H	2:C:175:ILE:HG13	1.70	0.41
2:C:209:PRO:O	2:C:213:ASN:HB2	2.20	0.41
1:E:29:GLU:C	1:E:31:GLY:H	2.23	0.41
1:F:96:PHE:HA	1:F:110:SER:HA	2.03	0.41
1:A:101:LEU:O	1:A:102:LYS:CG	2.68	0.41
2:G:112:LEU:O	2:G:113:SER:C	2.58	0.41
2:G:164:ILE:O	2:G:168:GLN:HG2	2.20	0.41
1:F:5:ILE:HG23	1:F:20:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:HIS:O	2:D:75:HIS:CD2	2.74	0.41
2:H:64:ARG:HH12	2:H:116:PRO:HG2	1.84	0.41
1:B:120:ALA:O	1:B:121:GLU:C	2.59	0.41
1:E:126:LEU:HD23	1:E:126:LEU:C	2.41	0.41
1:B:32:PHE:CD2	1:B:32:PHE:N	2.89	0.41
2:H:9:LEU:HD21	2:H:134:HIS:CD2	2.50	0.41
2:H:8:LEU:CD1	2:H:26:LYS:HG3	2.49	0.41
2:C:45:TRP:CZ3	2:C:104:LEU:HD12	2.56	0.41
1:F:88:PHE:CE1	1:F:93:CYS:O	2.74	0.41
1:F:37:THR:HG23	1:F:39:GLY:H	1.86	0.41
1:B:104:VAL:HA	2:C:68:PRO:CD	2.51	0.41
2:H:142:MET:HE3	2:H:218:TYR:N	2.36	0.41
2:H:97:CYS:HB2	2:H:106:LEU:CD1	2.49	0.41
2:C:170:SER:HB3	2:D:175:ILE:HG13	2.03	0.41
2:C:40:ASP:O	2:C:41:LEU:C	2.58	0.41
2:C:136:ILE:N	2:C:136:ILE:HD12	2.36	0.41
2:C:136:ILE:HG22	2:C:137:ARG:N	2.36	0.41
2:G:9:LEU:HG	2:G:134:HIS:CE1	2.56	0.41
2:C:198:LEU:N	2:C:199:PRO:HD2	2.36	0.41
1:F:81:ALA:O	1:F:82:ASP:O	2.39	0.41
1:B:120:ALA:HA	1:B:123:ILE:HD12	2.02	0.41
1:B:128:CYS:O	1:B:129:TYR:C	2.59	0.41
1:A:25:GLU:CG	1:A:26:LYS:N	2.84	0.41
2:G:217:LEU:O	2:G:221:VAL:HG23	2.21	0.41
2:G:43:GLN:HA	2:H:128:PRO:HB3	2.02	0.41
2:G:164:ILE:CG2	2:H:164:ILE:HG23	2.51	0.41
1:A:118:ASN:O	1:A:122:VAL:HG23	2.21	0.41
2:C:144:LEU:CA	2:D:214:LEU:HD11	2.50	0.41
2:C:167:TYR:HE1	2:D:174:LEU:HB2	1.86	0.41
1:A:124:ARG:NH2	1:B:16:ILE:HD12	2.36	0.41
1:B:9:HIS:NE2	1:B:14:PRO:O	2.50	0.41
1:B:122:VAL:O	1:B:125:GLU:CB	2.69	0.41
1:F:28:LEU:H	1:F:71:ARG:HH12	1.68	0.41
2:H:129:SER:O	2:H:133:GLN:HG2	2.21	0.41
1:B:99:LYS:HG2	1:B:100:ASN:H	1.84	0.40
2:D:1:MET:HG2	2:D:2:GLU:N	2.36	0.40
2:G:105:ILE:HG22	2:G:105:ILE:O	2.20	0.40
2:C:190:LEU:HD22	2:C:194:MET:HE3	2.03	0.40
2:G:152:GLU:OE2	2:H:197:LYS:HG3	2.21	0.40
1:B:1:MET:O	1:B:2:GLU:HG2	2.21	0.40
2:G:68:PRO:HA	2:G:69:PRO:HD3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:81:ARG:HB3	2:G:82:PRO:CD	2.33	0.40
2:C:75:HIS:NE2	2:C:117:PHE:HD2	2.19	0.40
1:F:120:ALA:HB1	1:F:124:ARG:NH1	2.35	0.40
2:G:63:LYS:O	2:G:65:LEU:N	2.55	0.40
2:C:167:TYR:HD2	2:D:167:TYR:CG	2.40	0.40
2:D:176:ARG:HB3	2:D:178:ARG:NH2	2.33	0.40
2:D:64:ARG:NH2	2:D:116:PRO:HB2	2.36	0.40
1:A:24:TRP:HB2	1:A:25:GLU:H	1.74	0.40
1:B:106:PHE:HB2	1:B:107:ARG:H	1.60	0.40
2:H:164:ILE:H	2:H:164:ILE:HG13	1.64	0.40
1:A:45:GLY:HA3	1:A:113:LEU:CD2	2.52	0.40
2:D:175:ILE:HG22	2:D:176:ARG:H	1.81	0.40
2:D:1:MET:CE	2:D:50:ASP:HB3	2.52	0.40
2:D:50:ASP:OD1	2:D:50:ASP:C	2.60	0.40
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.90	0.40
2:C:46:HIS:CE1	2:C:48:GLN:HG2	2.56	0.40
2:D:182:GLU:HG2	2:D:183:PRO:HD2	2.02	0.40
2:H:165:GLN:O	2:H:169:GLU:HG2	2.21	0.40
2:D:34:TYR:C	2:D:34:TYR:CD1	2.95	0.40
1:A:36:LEU:HG	1:A:36:LEU:O	2.20	0.40
2:H:142:MET:HE2	2:H:214:LEU:HB3	2.04	0.40
2:H:105:ILE:HA	2:H:121:PHE:O	2.22	0.40
2:D:207:GLY:O	2:D:210:PHE:HB3	2.22	0.40
2:G:136:ILE:HG12	2:H:135:LEU:HG	2.04	0.40
2:G:46:HIS:NE2	2:G:48:GLN:HG2	2.37	0.40
2:C:36:LEU:HD23	2:C:123:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	137/145 (94%)	95 (69%)	30 (22%)	12 (9%)	1	17
1	B	138/145 (95%)	95 (69%)	32 (23%)	11 (8%)	1	19
1	E	138/145 (95%)	121 (88%)	13 (9%)	4 (3%)	6	46
1	F	138/145 (95%)	113 (82%)	19 (14%)	6 (4%)	3	35
2	C	214/229 (93%)	175 (82%)	30 (14%)	9 (4%)	3	35
2	D	214/229 (93%)	166 (78%)	36 (17%)	12 (6%)	2	29
2	G	213/229 (93%)	170 (80%)	34 (16%)	9 (4%)	3	35
2	H	216/229 (94%)	151 (70%)	32 (15%)	33 (15%)	0	5
All	All	1408/1496 (94%)	1086 (77%)	226 (16%)	96 (7%)	1	24

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ALA
1	A	81	ALA
1	A	102	LYS
1	A	107	ARG
1	B	76	SER
1	B	93	CYS
1	B	104	VAL
1	B	105	SER
1	B	106	PHE
1	B	107	ARG
1	B	108	LEU
2	C	41	LEU
2	C	42	GLN
2	C	43	GLN
2	D	2	GLU
2	D	69	PRO
2	D	70	ALA
2	D	72	PHE
2	D	177	ASP
2	D	212	MET
1	E	107	ARG
1	E	108	LEU
1	F	82	ASP
1	F	93	CYS
1	F	107	ARG
1	F	108	LEU
2	G	64	ARG

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Mol	Chain	Res	Type
2	H	0	SER
2	H	2	GLU
2	H	3	GLU
2	H	4	LEU
2	H	5	GLU
2	H	6	GLN
2	H	8	LEU
2	H	10	MET
2	H	79	LEU
2	H	81	ARG
2	H	82	PRO
2	H	92	GLU
2	H	93	ALA
2	H	111	GLU
2	H	112	LEU
2	H	114	GLY
2	H	116	PRO
2	H	183	PRO
2	H	200	GLU
2	H	202	CYS
2	H	204	ILE
1	A	82	ASP
1	A	108	LEU
1	B	101	LEU
1	B	110	SER
2	C	32	GLN
2	D	172	ALA
2	D	205	GLY
1	E	60	ALA
1	F	94	TYR
2	G	61	LEU
2	G	62	ASN
2	H	1	MET
2	H	7	GLY
2	H	14	ALA
2	H	201	ALA
1	A	106	PHE
1	B	28	LEU
1	B	103	ASP
2	C	17	GLN
2	C	63	LYS
1	F	76	SER

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Mol	Chain	Res	Type
2	G	20	GLU
2	G	63	LYS
2	G	117	PHE
2	H	56	GLN
2	H	64	ARG
2	H	67	ALA
2	H	113	SER
2	H	177	ASP
1	A	103	ASP
1	A	118	ASN
2	C	93	ALA
2	D	66	THR
2	D	82	PRO
2	G	65	LEU
2	G	116	PRO
2	H	12	PRO
2	H	13	TRP
1	A	78	ALA
2	C	101	ALA
2	D	71	ALA
2	D	81	ARG
2	H	69	PRO
1	A	80	PRO
2	C	20	GLU
1	E	101	LEU
1	A	116	VAL
2	G	136	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	122/126 (97%)	96 (79%)	26 (21%)	1	11
1	B	123/126 (98%)	106 (86%)	17 (14%)	4	29
1	E	123/126 (98%)	104 (85%)	19 (15%)	3	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	123/126 (98%)	109 (89%)	14 (11%)	7	36
2	C	193/201 (96%)	168 (87%)	25 (13%)	5	31
2	D	189/201 (94%)	161 (85%)	28 (15%)	4	26
2	G	193/201 (96%)	162 (84%)	31 (16%)	3	22
2	H	193/201 (96%)	151 (78%)	42 (22%)	1	10
All	All	1259/1308 (96%)	1057 (84%)	202 (16%)	3	23

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	9	HIS
1	A	20	LEU
1	A	36	LEU
1	A	40	HIS
1	A	46	THR
1	A	47	VAL
1	A	51	GLU
1	A	58	ASP
1	A	69	GLU
1	A	70	LEU
1	A	71	ARG
1	A	72	LYS
1	A	83	VAL
1	A	85	THR
1	A	86	PHE
1	A	96	PHE
1	A	97	PHE
1	A	99	LYS
1	A	101	LEU
1	A	107	ARG
1	A	111	PHE
1	A	122	VAL
1	A	125	GLU
1	A	131	LEU
1	A	137	ASN
1	B	9	HIS
1	B	17	THR
1	B	36	LEU
1	B	46	THR

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Mol	Chain	Res	Type
1	B	63	LYS
1	B	82	ASP
1	B	85	THR
1	B	91	GLU
1	B	96	PHE
1	B	102	LYS
1	B	103	ASP
1	B	104	VAL
1	B	106	PHE
1	B	107	ARG
1	B	108	LEU
1	B	112	ASN
1	B	118	ASN
2	C	6	GLN
2	C	16	LEU
2	C	18	LEU
2	C	34	TYR
2	C	43	GLN
2	C	65	LEU
2	C	66	THR
2	C	73	LEU
2	C	75	HIS
2	C	78	ASN
2	C	83	LEU
2	C	94	THR
2	C	105	ILE
2	C	111	GLU
2	C	112	LEU
2	C	113	SER
2	C	135	LEU
2	C	157	LEU
2	C	161	ASP
2	C	175	ILE
2	C	177	ASP
2	C	185	GLU
2	C	187	ASN
2	C	200	GLU
2	C	206	ASP
2	D	6	GLN
2	D	29	ILE
2	D	34	TYR
2	D	43	GLN

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Mol	Chain	Res	Type
2	D	51	THR
2	D	65	LEU
2	D	72	PHE
2	D	80	LEU
2	D	94	THR
2	D	99	CYS
2	D	100	VAL
2	D	111	GLU
2	D	115	LEU
2	D	125	LEU
2	D	135	LEU
2	D	156	LEU
2	D	161	ASP
2	D	164	ILE
2	D	173	THR
2	D	175	ILE
2	D	176	ARG
2	D	178	ARG
2	D	179	LEU
2	D	185	GLU
2	D	208	LYS
2	D	213	ASN
2	D	218	TYR
2	D	222	THR
1	E	9	HIS
1	E	36	LEU
1	E	76	SER
1	E	82	ASP
1	E	84	TYR
1	E	86	PHE
1	E	91	GLU
1	E	95	PHE
1	E	96	PHE
1	E	97	PHE
1	E	102	LYS
1	E	103	ASP
1	E	106	PHE
1	E	107	ARG
1	E	108	LEU
1	E	112	ASN
1	E	116	VAL
1	E	121	GLU

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Mol	Chain	Res	Type
1	E	131	LEU
1	F	7	ARG
1	F	29	GLU
1	F	37	THR
1	F	57	ASP
1	F	58	ASP
1	F	63	LYS
1	F	70	LEU
1	F	89	SER
1	F	91	GLU
1	F	104	VAL
1	F	106	PHE
1	F	108	LEU
1	F	111	PHE
1	F	131	LEU
2	G	6	GLN
2	G	16	LEU
2	G	18	LEU
2	G	31	LYS
2	G	34	TYR
2	G	43	GLN
2	G	48	GLN
2	G	49	VAL
2	G	53	VAL
2	G	55	SER
2	G	56	GLN
2	G	57	ARG
2	G	59	LYS
2	G	60	GLU
2	G	61	LEU
2	G	63	LYS
2	G	84	LEU
2	G	94	THR
2	G	102	ASP
2	G	105	ILE
2	G	112	LEU
2	G	118	TYR
2	G	122	HIS
2	G	123	CYS
2	G	125	LEU
2	G	156	LEU
2	G	175	ILE

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Mol	Chain	Res	Type
2	G	185	GLU
2	G	187	ASN
2	G	206	ASP
2	G	222	THR
2	H	1	MET
2	H	2	GLU
2	H	6	GLN
2	H	8	LEU
2	H	10	MET
2	H	16	LEU
2	H	34	TYR
2	H	51	THR
2	H	61	LEU
2	H	63	LYS
2	H	65	LEU
2	H	66	THR
2	H	79	LEU
2	H	80	LEU
2	H	92	GLU
2	H	97	CYS
2	H	98	ASP
2	H	100	VAL
2	H	104	LEU
2	H	110	SER
2	H	111	GLU
2	H	112	LEU
2	H	115	LEU
2	H	121	PHE
2	H	132	SER
2	H	135	LEU
2	H	156	LEU
2	H	161	ASP
2	H	164	ILE
2	H	174	LEU
2	H	175	ILE
2	H	176	ARG
2	H	177	ASP
2	H	184	PHE
2	H	185	GLU
2	H	194	MET
2	H	200	GLU
2	H	206	ASP

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Mol	Chain	Res	Type
2	H	214	LEU
2	H	215	GLN
2	H	222	THR
2	H	224	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	118	ASN
2	C	6	GLN
2	C	46	HIS
2	C	48	GLN
2	C	147	GLN
2	C	187	ASN
2	C	224	GLN
2	D	6	GLN
2	D	75	HIS
2	D	122	HIS
1	F	112	ASN
1	F	118	ASN
2	G	120	ASN
2	G	149	GLN
2	G	213	ASN
2	H	6	GLN
2	H	32	GLN
2	H	75	HIS
2	H	134	HIS
2	H	149	GLN
2	H	224	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	139/145 (95%)	-0.21	1 (0%) 89 84	80, 80, 80, 80	0
1	B	140/145 (96%)	0.02	8 (5%) 27 19	80, 80, 80, 80	0
1	E	140/145 (96%)	-0.03	3 (2%) 67 56	80, 80, 80, 80	0
1	F	140/145 (96%)	0.07	10 (7%) 19 13	80, 80, 80, 80	0
2	C	218/229 (95%)	0.02	3 (1%) 78 68	80, 80, 80, 80	0
2	D	218/229 (95%)	-0.02	3 (1%) 78 68	80, 80, 80, 80	0
2	G	217/229 (94%)	0.13	7 (3%) 51 38	80, 80, 80, 80	0
2	H	220/229 (96%)	-0.04	4 (1%) 71 61	80, 80, 80, 80	0
All	All	1432/1496 (95%)	-0.00	39 (2%) 58 46	80, 80, 80, 80	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	74	LEU	4.2
1	A	75	LEU	3.6
2	G	120	ASN	3.6
2	D	173	THR	3.5
2	G	23	LEU	3.5
1	E	63	LYS	3.5
1	B	8	ILE	3.3
1	F	36	LEU	3.1
1	B	19	PHE	3.1
1	B	86	PHE	3.1
1	B	108	LEU	3.0
2	H	112	LEU	3.0
2	G	119	TRP	2.9
1	F	108	LEU	2.9
2	H	13	TRP	2.8
1	E	137	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	111	PHE	2.6
1	F	69	GLU	2.6
1	B	18	HIS	2.5
2	D	157	LEU	2.5
1	B	32	PHE	2.3
1	F	8	ILE	2.3
1	F	43	TRP	2.3
1	E	74	LEU	2.3
2	G	115	LEU	2.2
2	C	116	PRO	2.2
2	H	21	ASN	2.2
1	B	90	LYS	2.2
1	F	19	PHE	2.2
2	C	119	TRP	2.2
2	D	140	MET	2.1
2	C	184	PHE	2.1
1	F	106	PHE	2.1
1	F	73	ALA	2.1
2	H	23	LEU	2.1
2	G	73	LEU	2.1
1	B	42	ALA	2.0
2	G	194	MET	2.0
2	G	153	LEU	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.