



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 11:44 AM EDT

PDB ID : 2G33  
Title : Human Hepatitis B Virus T=4 capsid, strain adyw  
Authors : Bourne, C.R.; Zlotnick, A.  
Deposited on : unknown  
Resolution : 3.96 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

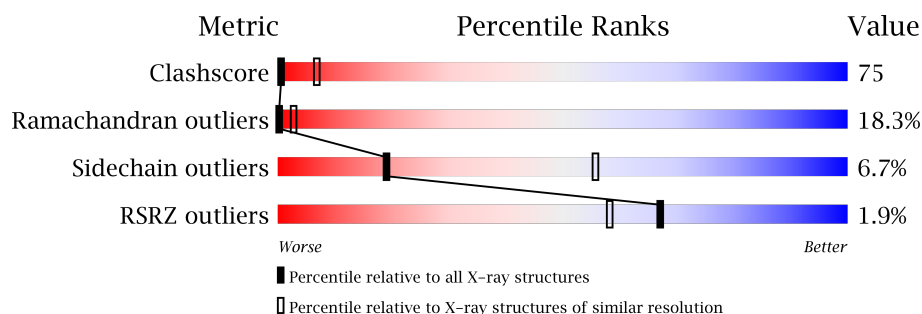
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.96 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))
Clashscore	112137	1154 (4.32-3.60)
Ramachandran outliers	110173	1111 (4.32-3.60)
Sidechain outliers	110143	1101 (4.32-3.60)
RSRZ outliers	101464	1069 (4.32-3.60)

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	150	
1	B	150	
1	C	150	
1	D	150	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4658 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 Core antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	147	Total	C	N	O	S	0	0	0
			1167	759	191	215	2			
1	D	146	Total	C	N	O	S	0	0	0
			1160	755	190	213	2			
1	B	147	Total	C	N	O	S	0	0	0
			1167	759	191	215	2			
1	A	148	Total	C	N	O	S	0	0	0
			1164	758	192	212	2			

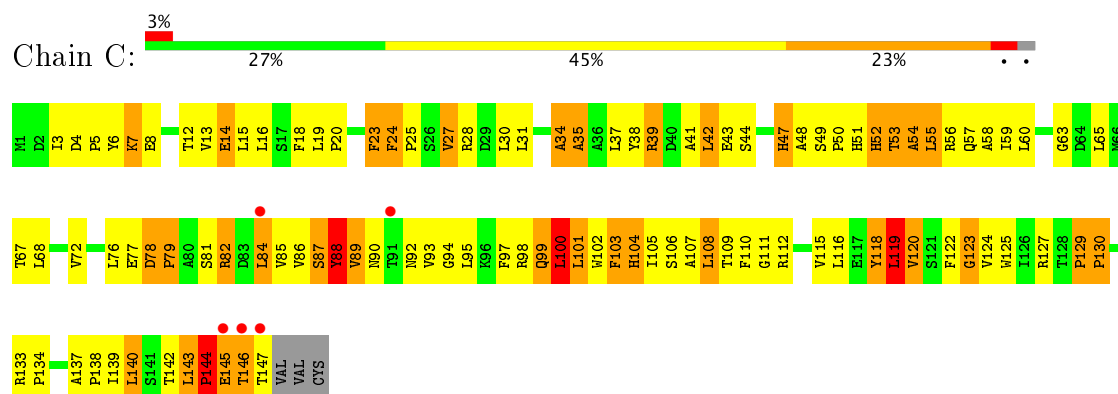
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	ALA	CYS	ENGINEERED	UNP P03147
C	61	ALA	CYS	ENGINEERED	UNP P03147
C	107	ALA	CYS	ENGINEERED	UNP P03147
C	150	CYS	-	INSERTION	UNP P03147
D	48	ALA	CYS	ENGINEERED	UNP P03147
D	61	ALA	CYS	ENGINEERED	UNP P03147
D	107	ALA	CYS	ENGINEERED	UNP P03147
D	150	CYS	-	INSERTION	UNP P03147
B	48	ALA	CYS	ENGINEERED	UNP P03147
B	61	ALA	CYS	ENGINEERED	UNP P03147
B	107	ALA	CYS	ENGINEERED	UNP P03147
B	150	CYS	-	INSERTION	UNP P03147
A	48	ALA	CYS	ENGINEERED	UNP P03147
A	61	ALA	CYS	ENGINEERED	UNP P03147
A	107	ALA	CYS	ENGINEERED	UNP P03147
A	150	CYS	-	INSERTION	UNP P03147

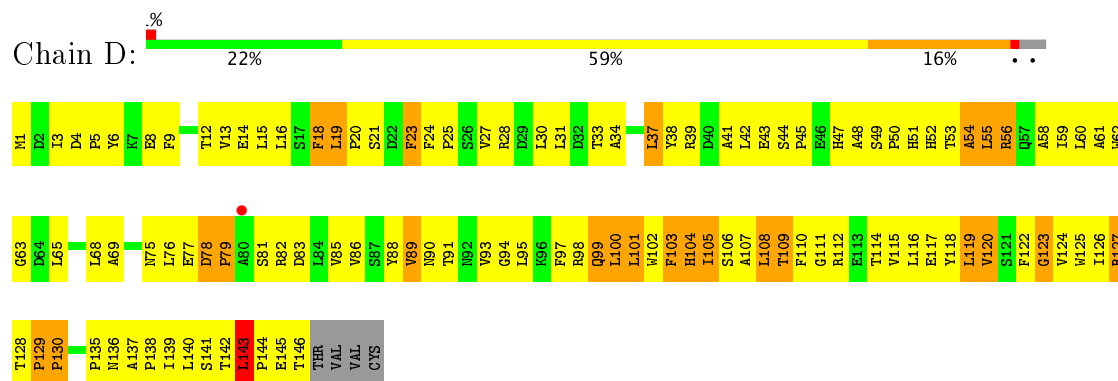
### 3 Residue-property plots [i](#)

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

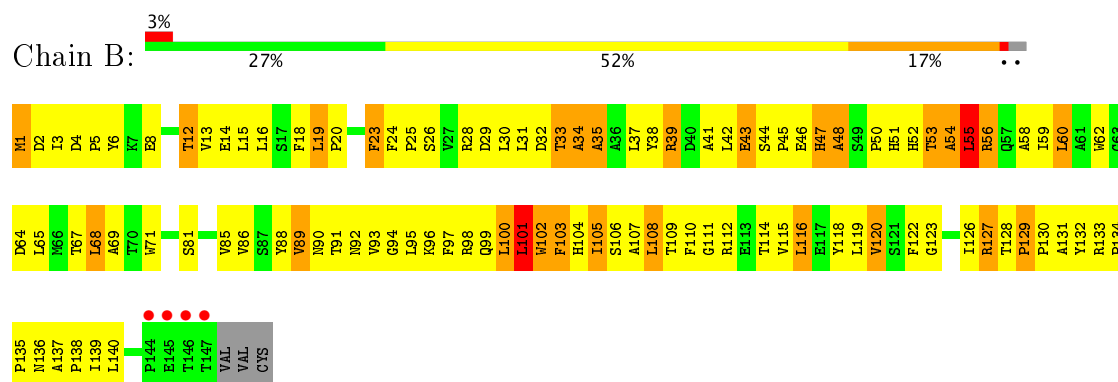
#### • Molecule 1: Core antigen



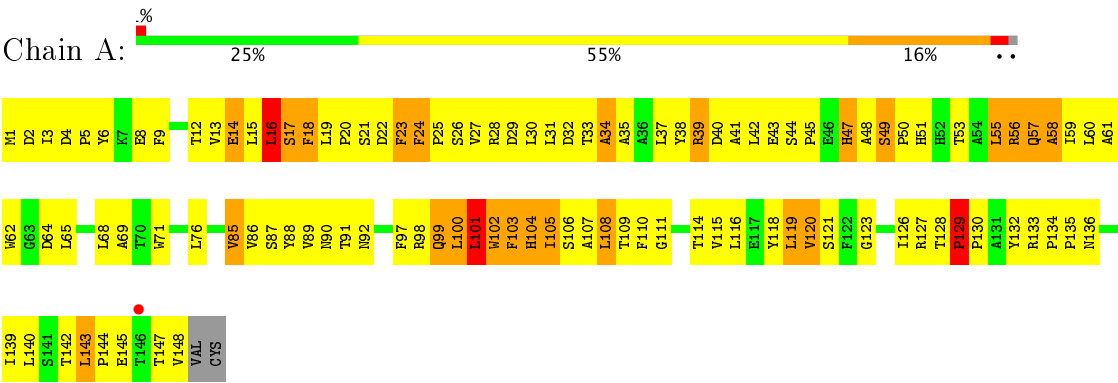
#### • Molecule 1: Core antigen



#### • Molecule 1: Core antigen



● Molecule 1: Core antigen



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	558.40Å 327.14Å 562.24Å 90.00° 109.12° 90.00°	Depositor
Resolution (Å)	40.00 – 3.96 39.95 – 4.00	Depositor EDS
% Data completeness (in resolution range)	79.2 (40.00-3.96) 81.5 (39.95-4.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 4.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.360 , 0.372 0.334 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	133.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	4658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.62	0/1200	0.88	1/1648 (0.1%)
1	B	0.64	0/1203	0.86	1/1652 (0.1%)
1	C	0.62	0/1203	0.98	6/1652 (0.4%)
1	D	0.66	0/1196	0.92	1/1642 (0.1%)
All	All	0.63	0/4802	0.91	9/6594 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	GLU	N-CA-C	9.47	136.58	111.00
1	C	144	PRO	N-CA-C	7.60	131.85	112.10
1	D	143	LEU	N-CA-C	7.07	130.09	111.00
1	C	82	ARG	N-CA-C	-6.53	93.37	111.00
1	C	140	LEU	N-CA-C	5.73	126.46	111.00
1	C	100	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	60	LEU	CA-CB-CG	-5.53	102.58	115.30
1	A	16	LEU	CA-CB-CG	-5.12	103.53	115.30
1	C	42	LEU	CA-CB-CG	-5.07	103.64	115.30

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	1164	0	1136	187	0
1	B	1167	0	1148	166	0
1	C	1167	0	1148	199	0
1	D	1160	0	1141	195	0
All	All	4658	0	4573	696	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 75.

All (696) 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:139:ILE:HG22	1:A:140:LEU:H	0.93	1.07
1:C:78:ASP:HB3	1:C:79:PRO:CD	1.80	1.06
1:D:139:ILE:HG22	1:D:140:LEU:H	1.18	1.04
1:C:78:ASP:HB3	1:C:79:PRO:HD3	1.10	1.04
1:D:55:LEU:HD12	1:D:55:LEU:H	1.25	1.01
1:D:12:THR:HG23	1:D:15:LEU:HB2	1.41	1.00
1:A:139:ILE:CG2	1:A:140:LEU:H	1.74	0.98
1:C:3:ILE:HG22	1:D:43:GLU:HG2	1.46	0.97
1:C:129:PRO:HG2	1:B:23:PHE:O	1.63	0.97
1:A:139:ILE:HG22	1:A:140:LEU:N	1.74	0.96
1:D:119:LEU:HD12	1:D:119:LEU:H	1.31	0.96
1:A:119:LEU:HD12	1:A:119:LEU:H	1.27	0.96
1:B:55:LEU:HG	1:B:59:ILE:HD11	1.48	0.95
1:D:116:LEU:O	1:D:120:VAL:HG23	1.64	0.95
1:C:12:THR:HG23	1:C:15:LEU:HB2	1.48	0.94
1:B:119:LEU:HD12	1:B:119:LEU:H	1.30	0.93
1:C:119:LEU:HD12	1:C:119:LEU:H	1.30	0.93
1:B:110:PHE:O	1:B:114:THR:HB	1.68	0.92
1:B:59:ILE:H	1:B:59:ILE:HD12	1.34	0.92
1:C:100:LEU:O	1:C:103:PHE:HB3	1.71	0.90
1:A:15:LEU:HD22	1:A:16:LEU:HD23	1.51	0.89
1:C:24:PHE:H	1:C:24:PHE:HD2	1.16	0.89
1:D:15:LEU:HD21	1:D:119:LEU:HD23	1.54	0.88
1:C:118:TYR:HD1	1:C:140:LEU:HD21	1.36	0.88
1:B:60:LEU:HD12	1:A:5:PRO:HG3	1.56	0.87
1:C:116:LEU:O	1:C:120:VAL:HG23	1.75	0.87
1:C:51:HIS:HB3	1:C:108:LEU:HD11	1.57	0.87
1:C:15:LEU:HD21	1:C:119:LEU:HD23	1.54	0.87
1:B:42:LEU:C	1:B:44:SER:H	1.78	0.86
1:C:118:TYR:CD1	1:C:140:LEU:HD21	2.09	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:O	1:B:120:VAL:HG23	1.75	0.86
1:A:100:LEU:HD23	1:A:101:LEU:N	1.90	0.85
1:D:12:THR:O	1:D:15:LEU:HB3	1.76	0.85
1:C:18:PHE:HE1	1:B:33:THR:HA	1.40	0.85
1:A:12:THR:O	1:A:15:LEU:HB3	1.77	0.85
1:D:139:ILE:HG22	1:D:140:LEU:N	1.92	0.83
1:C:18:PHE:HE2	1:C:123:GLY:HA3	1.44	0.83
1:A:100:LEU:O	1:A:103:PHE:HB3	1.78	0.83
1:D:119:LEU:H	1:D:119:LEU:CD1	1.92	0.83
1:D:23:PHE:HD2	1:D:23:PHE:C	1.82	0.83
1:C:13:VAL:HG13	1:C:14:GLU:H	1.45	0.82
1:B:12:THR:HG23	1:B:15:LEU:HB2	1.60	0.82
1:C:59:ILE:H	1:C:59:ILE:HD12	1.45	0.82
1:D:110:PHE:O	1:D:114:THR:HB	1.80	0.81
1:C:60:LEU:HD11	1:D:3:ILE:HD11	1.61	0.81
1:C:89:VAL:HA	1:C:93:VAL:HG12	1.62	0.81
1:A:119:LEU:N	1:A:119:LEU:HD12	1.94	0.81
1:B:100:LEU:O	1:B:103:PHE:HB3	1.80	0.81
1:D:42:LEU:C	1:D:44:SER:H	1.82	0.81
1:D:78:ASP:HB2	1:D:79:PRO:CD	2.10	0.80
1:D:97:PHE:O	1:D:101:LEU:HB2	1.82	0.80
1:D:100:LEU:HD23	1:D:101:LEU:N	1.96	0.80
1:C:47:HIS:HB3	1:D:8:GLU:OE2	1.82	0.80
1:C:55:LEU:HD23	1:C:56:ARG:N	1.96	0.79
1:C:24:PHE:HD2	1:C:24:PHE:N	1.78	0.78
1:D:139:ILE:CG2	1:D:140:LEU:H	1.95	0.78
1:B:62:TRP:HB2	1:B:97:PHE:CE2	2.19	0.78
1:D:89:VAL:HA	1:D:93:VAL:HG12	1.66	0.78
1:D:145:GLU:HG3	1:D:146:THR:H	1.47	0.77
1:D:23:PHE:CD2	1:D:23:PHE:C	2.56	0.77
1:B:23:PHE:HD2	1:B:23:PHE:C	1.87	0.77
1:C:13:VAL:HG13	1:C:14:GLU:N	2.00	0.76
1:C:110:PHE:CE2	1:C:140:LEU:HB3	2.21	0.76
1:B:35:ALA:O	1:B:39:ARG:HB2	1.86	0.76
1:C:27:VAL:HG12	1:C:31:LEU:HD11	1.68	0.76
1:C:8:GLU:HG3	1:D:47:HIS:HB3	1.68	0.75
1:D:51:HIS:HB3	1:D:108:LEU:HD11	1.69	0.75
1:D:59:ILE:H	1:D:59:ILE:HD12	1.51	0.75
1:B:39:ARG:NH2	1:A:1:MET:HB2	2.01	0.75
1:A:89:VAL:C	1:A:91:THR:H	1.90	0.75
1:C:15:LEU:HD23	1:C:15:LEU:C	2.07	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PHE:CE2	1:C:123:GLY:HA3	2.20	0.75
1:C:23:PHE:C	1:C:23:PHE:CD1	2.60	0.74
1:A:42:LEU:C	1:A:44:SER:H	1.89	0.74
1:C:24:PHE:CD2	1:C:24:PHE:N	2.52	0.74
1:D:55:LEU:H	1:D:55:LEU:CD1	2.00	0.74
1:D:77:GLU:HA	1:D:82:ARG:HD3	1.70	0.74
1:A:47:HIS:O	1:A:49:SER:N	2.21	0.73
1:A:126:ILE:HG23	1:A:127:ARG:H	1.54	0.73
1:B:12:THR:O	1:B:15:LEU:HB3	1.88	0.73
1:B:23:PHE:C	1:B:23:PHE:CD2	2.60	0.73
1:D:15:LEU:CD2	1:D:119:LEU:HD23	2.19	0.73
1:C:95:LEU:O	1:C:99:GLN:HB2	1.89	0.72
1:D:138:PRO:C	1:D:139:ILE:HG13	2.07	0.72
1:B:56:ARG:HA	1:B:59:ILE:HD13	1.69	0.72
1:B:81:SER:HB2	1:A:76:LEU:HD21	1.71	0.72
1:C:60:LEU:HD13	1:D:5:PRO:HG3	1.71	0.72
1:C:109:THR:HB	1:C:110:PHE:CD1	2.25	0.72
1:A:51:HIS:HB3	1:A:108:LEU:HD11	1.71	0.71
1:B:19:LEU:HD23	1:B:19:LEU:N	2.03	0.71
1:B:59:ILE:N	1:B:59:ILE:HD12	2.06	0.71
1:D:126:ILE:C	1:D:128:THR:H	1.92	0.71
1:D:21:SER:HB3	1:D:95:LEU:HD11	1.71	0.71
1:A:123:GLY:O	1:A:127:ARG:HG2	1.91	0.71
1:A:55:LEU:HB3	1:A:59:ILE:HD11	1.73	0.70
1:A:23:PHE:CD2	1:A:23:PHE:C	2.64	0.70
1:D:78:ASP:HB2	1:D:79:PRO:HD2	1.72	0.70
1:A:109:THR:HB	1:A:110:PHE:CD2	2.26	0.70
1:A:4:ASP:OD2	1:A:13:VAL:HG12	1.91	0.70
1:C:109:THR:HB	1:C:110:PHE:CE1	2.27	0.69
1:A:142:THR:O	1:A:144:PRO:HD3	1.91	0.69
1:C:5:PRO:HG3	1:D:60:LEU:HD12	1.72	0.69
1:C:120:VAL:O	1:C:124:VAL:HG23	1.93	0.69
1:C:47:HIS:O	1:C:49:SER:N	2.25	0.69
1:D:75:ASN:O	1:D:76:LEU:HG	1.92	0.69
1:B:39:ARG:HH21	1:A:1:MET:HB2	1.56	0.69
1:C:12:THR:O	1:C:15:LEU:HB3	1.92	0.69
1:C:81:SER:OG	1:D:76:LEU:HD21	1.91	0.69
1:C:78:ASP:CB	1:C:79:PRO:CD	2.65	0.68
1:C:122:PHE:O	1:C:125:TRP:N	2.24	0.68
1:B:62:TRP:HB2	1:B:97:PHE:HE2	1.58	0.68
1:B:5:PRO:HB3	1:A:60:LEU:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:O	1:C:18:PHE:HB2	1.94	0.67
1:B:42:LEU:HA	1:B:56:ARG:HH21	1.59	0.67
1:C:85:VAL:O	1:C:89:VAL:HG23	1.94	0.67
1:B:25:PRO:O	1:B:98:ARG:HD2	1.94	0.67
1:C:42:LEU:C	1:C:44:SER:H	1.98	0.67
1:A:13:VAL:C	1:A:15:LEU:N	2.47	0.67
1:B:119:LEU:CD1	1:B:119:LEU:H	2.07	0.67
1:B:85:VAL:HG23	1:B:86:VAL:N	2.10	0.67
1:A:1:MET:HG3	1:A:3:ILE:HG23	1.77	0.66
1:B:60:LEU:HG	1:A:3:ILE:HD11	1.77	0.66
1:B:60:LEU:CD1	1:A:5:PRO:HG3	2.23	0.66
1:C:23:PHE:HD1	1:C:24:PHE:N	1.94	0.66
1:A:33:THR:HG22	1:A:34:ALA:N	2.09	0.66
1:C:18:PHE:HE2	1:C:123:GLY:CA	2.08	0.66
1:C:23:PHE:HD1	1:C:23:PHE:C	1.99	0.66
1:C:25:PRO:HB2	1:C:30:LEU:HD11	1.77	0.66
1:A:55:LEU:HD11	1:A:104:HIS:HB3	1.78	0.66
1:B:47:HIS:HD2	1:A:50:PRO:HG2	1.59	0.66
1:D:102:TRP:O	1:D:103:PHE:C	2.34	0.66
1:C:24:PHE:CD1	1:C:99:GLN:HA	2.31	0.65
1:B:15:LEU:HD22	1:B:16:LEU:HD23	1.79	0.65
1:C:72:VAL:HG12	1:C:72:VAL:O	1.96	0.65
1:A:109:THR:HB	1:A:110:PHE:CE2	2.31	0.65
1:D:12:THR:CG2	1:D:15:LEU:HB2	2.22	0.65
1:D:59:ILE:HD12	1:D:59:ILE:N	2.10	0.65
1:B:100:LEU:HD23	1:B:100:LEU:C	2.18	0.64
1:C:38:TYR:O	1:C:41:ALA:N	2.30	0.64
1:D:122:PHE:C	1:D:124:VAL:H	1.99	0.64
1:D:126:ILE:O	1:D:128:THR:N	2.31	0.64
1:A:13:VAL:C	1:A:15:LEU:H	2.01	0.64
1:B:47:HIS:HB3	1:A:8:GLU:OE1	1.96	0.64
1:C:146:THR:O	1:C:147:THR:O	2.15	0.64
1:A:111:GLY:O	1:A:115:VAL:HG23	1.98	0.64
1:B:115:VAL:O	1:B:118:TYR:HB3	1.98	0.64
1:B:3:ILE:HG22	1:A:43:GLU:HG2	1.80	0.64
1:A:116:LEU:O	1:A:120:VAL:HG23	1.97	0.64
1:D:126:ILE:HG23	1:D:127:ARG:H	1.61	0.64
1:A:118:TYR:O	1:A:119:LEU:C	2.35	0.64
1:B:100:LEU:CD2	1:B:101:LEU:N	2.61	0.64
1:D:4:ASP:OD2	1:D:13:VAL:HG12	1.98	0.63
1:C:139:ILE:HG22	1:C:140:LEU:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:C	1:B:15:LEU:N	2.48	0.63
1:D:85:VAL:O	1:D:89:VAL:HG23	1.99	0.63
1:C:13:VAL:CG1	1:C:14:GLU:H	2.10	0.63
1:D:3:ILE:C	1:D:3:ILE:HD12	2.19	0.63
1:C:79:PRO:HG2	1:D:78:ASP:CG	2.19	0.63
1:B:55:LEU:HG	1:B:59:ILE:CD1	2.25	0.63
1:B:42:LEU:C	1:B:44:SER:N	2.48	0.63
1:C:59:ILE:HD12	1:C:59:ILE:N	2.13	0.63
1:A:132:TYR:O	1:A:134:PRO:HD3	1.98	0.63
1:C:15:LEU:O	1:C:18:PHE:CB	2.47	0.63
1:D:135:PRO:HG2	1:D:136:ASN:H	1.62	0.63
1:D:18:PHE:CE1	1:D:123:GLY:HA3	2.34	0.63
1:A:55:LEU:C	1:A:59:ILE:HD12	2.19	0.62
1:A:126:ILE:HG23	1:A:127:ARG:N	2.13	0.62
1:B:107:ALA:C	1:B:109:THR:H	2.03	0.62
1:A:15:LEU:HD23	1:A:15:LEU:C	2.20	0.62
1:B:59:ILE:H	1:B:59:ILE:CD1	2.09	0.62
1:C:38:TYR:O	1:C:39:ARG:C	2.37	0.62
1:C:60:LEU:CD1	1:D:5:PRO:HG3	2.30	0.62
1:D:16:LEU:C	1:D:18:PHE:N	2.47	0.62
1:C:122:PHE:O	1:C:124:VAL:N	2.33	0.62
1:A:12:THR:HG23	1:A:15:LEU:HB2	1.80	0.62
1:D:15:LEU:O	1:D:15:LEU:HD23	1.99	0.62
1:D:78:ASP:CB	1:D:79:PRO:CD	2.77	0.62
1:A:143:LEU:C	1:A:145:GLU:H	2.03	0.62
1:B:139:ILE:HG22	1:B:140:LEU:H	1.64	0.62
1:B:53:THR:HG23	1:A:8:GLU:OE1	2.00	0.62
1:C:4:ASP:OD2	1:C:13:VAL:HG12	2.00	0.61
1:D:116:LEU:N	1:D:116:LEU:HD23	2.14	0.61
1:D:12:THR:HG23	1:D:15:LEU:CB	2.26	0.61
1:D:141:SER:C	1:D:143:LEU:H	2.04	0.61
1:A:102:TRP:O	1:A:103:PHE:C	2.39	0.61
1:C:100:LEU:HD23	1:C:100:LEU:C	2.21	0.61
1:C:12:THR:HG23	1:C:15:LEU:CB	2.26	0.61
1:B:23:PHE:O	1:B:23:PHE:HD2	1.81	0.61
1:C:103:PHE:CD2	1:C:104:HIS:N	2.68	0.61
1:D:145:GLU:HG3	1:D:146:THR:N	2.15	0.61
1:D:47:HIS:O	1:D:49:SER:N	2.34	0.61
1:D:145:GLU:CG	1:D:146:THR:N	2.64	0.61
1:C:15:LEU:HD22	1:C:16:LEU:HD23	1.83	0.61
1:C:15:LEU:CD2	1:C:16:LEU:HD23	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:O	1:A:15:LEU:N	2.33	0.60
1:B:115:VAL:O	1:B:118:TYR:N	2.30	0.60
1:C:3:ILE:C	1:C:3:ILE:HD12	2.20	0.60
1:B:67:THR:O	1:B:67:THR:HG22	2.01	0.60
1:A:13:VAL:HG13	1:A:14:GLU:N	2.17	0.60
1:A:15:LEU:CD2	1:A:16:LEU:N	2.64	0.60
1:D:93:VAL:HG13	1:D:94:GLY:N	2.16	0.60
1:D:55:LEU:HD12	1:D:55:LEU:N	2.03	0.60
1:D:51:HIS:CB	1:D:108:LEU:HD11	2.32	0.60
1:B:56:ARG:CA	1:B:59:ILE:HD13	2.32	0.60
1:D:119:LEU:HD12	1:D:119:LEU:N	2.08	0.60
1:B:106:SER:O	1:B:110:PHE:HD2	1.82	0.60
1:D:15:LEU:HD21	1:D:119:LEU:CD2	2.28	0.60
1:D:51:HIS:HB3	1:D:108:LEU:CD1	2.32	0.60
1:A:23:PHE:HD2	1:A:23:PHE:C	2.04	0.60
1:C:119:LEU:HD12	1:C:119:LEU:N	2.11	0.60
1:C:76:LEU:O	1:C:82:ARG:HD3	2.02	0.60
1:D:112:ARG:O	1:D:115:VAL:HB	2.02	0.60
1:A:118:TYR:CE2	1:A:140:LEU:HG	2.37	0.59
1:B:5:PRO:HB3	1:A:60:LEU:CD1	2.32	0.59
1:D:13:VAL:HG13	1:D:14:GLU:N	2.17	0.59
1:A:89:VAL:C	1:A:91:THR:N	2.55	0.59
1:C:139:ILE:CG2	1:C:140:LEU:N	2.65	0.59
1:A:107:ALA:C	1:A:109:THR:H	2.06	0.59
1:A:42:LEU:C	1:A:44:SER:N	2.55	0.59
1:B:43:GLU:HG2	1:A:3:ILE:HG22	1.84	0.59
1:D:93:VAL:C	1:D:95:LEU:N	2.55	0.59
1:C:24:PHE:CE1	1:C:99:GLN:HG3	2.37	0.59
1:D:59:ILE:H	1:D:59:ILE:CD1	2.15	0.59
1:A:20:PRO:C	1:A:22:ASP:H	2.03	0.59
1:B:100:LEU:HD23	1:B:101:LEU:N	2.18	0.59
1:C:59:ILE:CD1	1:C:59:ILE:H	2.13	0.59
1:D:15:LEU:O	1:D:16:LEU:HD23	2.02	0.59
1:A:115:VAL:O	1:A:118:TYR:N	2.31	0.59
1:A:119:LEU:N	1:A:119:LEU:CD1	2.65	0.59
1:A:87:SER:O	1:A:91:THR:HB	2.02	0.59
1:C:35:ALA:CB	1:D:1:MET:HE1	2.32	0.59
1:A:55:LEU:HB3	1:A:59:ILE:CD1	2.33	0.59
1:A:143:LEU:C	1:A:145:GLU:N	2.52	0.58
1:C:12:THR:CG2	1:C:15:LEU:HB2	2.28	0.58
1:C:88:TYR:O	1:C:92:ASN:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:C	1:D:100:LEU:HD23	2.24	0.58
1:D:137:ALA:HB1	1:D:138:PRO:HD2	1.85	0.58
1:D:42:LEU:C	1:D:44:SER:N	2.51	0.58
1:D:6:TYR:C	1:D:8:GLU:N	2.57	0.58
1:C:24:PHE:CE1	1:C:99:GLN:HA	2.38	0.58
1:A:23:PHE:O	1:A:23:PHE:HD2	1.87	0.58
1:B:103:PHE:CD2	1:B:104:HIS:N	2.71	0.58
1:C:107:ALA:C	1:C:109:THR:H	2.07	0.58
1:A:16:LEU:O	1:A:18:PHE:N	2.36	0.58
1:A:26:SER:O	1:A:29:ASP:HB2	2.04	0.58
1:A:89:VAL:O	1:A:91:THR:N	2.37	0.58
1:C:139:ILE:HG23	1:C:140:LEU:HG	1.85	0.58
1:D:59:ILE:O	1:D:63:GLY:N	2.34	0.58
1:C:4:ASP:OD1	1:C:6:TYR:HD2	1.87	0.58
1:B:68:LEU:HD13	1:A:88:TYR:CE2	2.38	0.57
1:A:119:LEU:O	1:A:120:VAL:C	2.43	0.57
1:B:139:ILE:HG22	1:B:140:LEU:N	2.19	0.57
1:A:24:PHE:N	1:A:24:PHE:CD1	2.66	0.57
1:C:100:LEU:HD23	1:C:101:LEU:N	2.18	0.57
1:C:51:HIS:CB	1:C:108:LEU:HD11	2.33	0.57
1:A:15:LEU:HD22	1:A:16:LEU:CD2	2.31	0.57
1:D:13:VAL:C	1:D:15:LEU:N	2.57	0.57
1:C:5:PRO:HG3	1:D:60:LEU:CD1	2.35	0.57
1:C:127:ARG:HD2	1:B:29:ASP:HB3	1.87	0.57
1:C:37:LEU:HD12	1:C:37:LEU:O	2.05	0.57
1:D:109:THR:HB	1:D:110:PHE:CE1	2.39	0.57
1:C:119:LEU:H	1:C:119:LEU:CD1	2.09	0.57
1:D:23:PHE:HD2	1:D:23:PHE:O	1.86	0.57
1:D:19:LEU:HD23	1:D:19:LEU:N	2.20	0.57
1:B:106:SER:O	1:B:110:PHE:CD2	2.57	0.57
1:D:126:ILE:HG23	1:D:127:ARG:N	2.19	0.57
1:D:16:LEU:C	1:D:18:PHE:H	2.07	0.57
1:D:30:LEU:O	1:D:33:THR:HB	2.05	0.57
1:B:38:TYR:HB2	1:B:42:LEU:HD11	1.86	0.57
1:C:88:TYR:O	1:C:92:ASN:N	2.31	0.56
1:C:118:TYR:HB3	1:C:119:LEU:HD12	1.86	0.56
1:C:55:LEU:O	1:C:58:ALA:HB3	2.05	0.56
1:A:20:PRO:C	1:A:22:ASP:N	2.59	0.56
1:B:85:VAL:CG2	1:B:86:VAL:N	2.67	0.56
1:C:130:PRO:O	1:C:133:ARG:HG2	2.06	0.56
1:A:100:LEU:CD2	1:A:101:LEU:N	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:VAL:HG23	1:D:86:VAL:HG23	1.88	0.56
1:C:53:THR:HG23	1:D:8:GLU:OE2	2.06	0.56
1:A:101:LEU:O	1:A:102:TRP:C	2.42	0.56
1:B:15:LEU:O	1:B:15:LEU:HD23	2.04	0.56
1:D:126:ILE:C	1:D:128:THR:N	2.59	0.56
1:D:55:LEU:O	1:D:58:ALA:N	2.39	0.56
1:A:116:LEU:O	1:A:120:VAL:CG2	2.53	0.56
1:B:128:THR:O	1:B:133:ARG:NH1	2.38	0.56
1:A:142:THR:HG22	1:A:143:LEU:N	2.21	0.55
1:C:8:GLU:CG	1:D:47:HIS:HB3	2.35	0.55
1:B:4:ASP:OD2	1:B:13:VAL:HG12	2.07	0.55
1:B:89:VAL:O	1:B:91:THR:N	2.39	0.55
1:B:122:PHE:O	1:B:123:GLY:C	2.44	0.55
1:B:13:VAL:C	1:B:15:LEU:H	2.09	0.55
1:C:16:LEU:C	1:C:18:PHE:H	2.09	0.55
1:A:100:LEU:O	1:A:101:LEU:C	2.44	0.55
1:C:100:LEU:CD2	1:C:101:LEU:N	2.69	0.55
1:A:56:ARG:HB2	1:A:57:GLN:NE2	2.21	0.55
1:C:115:VAL:O	1:C:118:TYR:N	2.39	0.55
1:C:6:TYR:O	1:C:8:GLU:N	2.40	0.55
1:D:86:VAL:HA	1:D:89:VAL:HB	1.88	0.55
1:C:129:PRO:HB3	1:C:130:PRO:HD2	1.89	0.55
1:A:34:ALA:O	1:A:37:LEU:HB3	2.07	0.55
1:B:81:SER:CB	1:A:76:LEU:HD21	2.36	0.55
1:D:122:PHE:O	1:D:124:VAL:N	2.40	0.54
1:D:122:PHE:O	1:D:126:ILE:HG22	2.07	0.54
1:D:15:LEU:HD23	1:D:16:LEU:CD2	2.37	0.54
1:A:61:ALA:O	1:A:64:ASP:HB2	2.07	0.54
1:C:82:ARG:HB2	1:C:82:ARG:HH11	1.72	0.54
1:D:115:VAL:O	1:D:118:TYR:CB	2.56	0.54
1:D:30:LEU:HD23	1:D:101:LEU:HD22	1.89	0.54
1:A:12:THR:CG2	1:A:15:LEU:HB2	2.36	0.54
1:B:38:TYR:O	1:B:41:ALA:N	2.40	0.54
1:C:16:LEU:C	1:C:18:PHE:N	2.60	0.54
1:C:23:PHE:CD1	1:C:24:PHE:N	2.76	0.54
1:D:110:PHE:CE2	1:D:140:LEU:HB3	2.42	0.54
1:C:60:LEU:HD11	1:D:3:ILE:CD1	2.36	0.54
1:D:18:PHE:CD1	1:D:123:GLY:HA3	2.42	0.54
1:D:13:VAL:C	1:D:15:LEU:H	2.09	0.54
1:D:99:GLN:O	1:D:100:LEU:C	2.45	0.54
1:C:15:LEU:HD21	1:C:119:LEU:CD2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:TYR:C	1:C:8:GLU:N	2.57	0.54
1:D:61:ALA:O	1:D:65:LEU:HG	2.08	0.54
1:A:107:ALA:O	1:A:109:THR:N	2.39	0.54
1:B:112:ARG:O	1:B:115:VAL:HB	2.07	0.54
1:B:94:GLY:O	1:B:98:ARG:HG3	2.07	0.54
1:C:41:ALA:O	1:C:44:SER:HB3	2.08	0.53
1:C:67:THR:HG22	1:C:67:THR:O	2.08	0.53
1:D:13:VAL:HG13	1:D:14:GLU:H	1.72	0.53
1:A:103:PHE:CD2	1:A:104:HIS:N	2.76	0.53
1:D:100:LEU:CD2	1:D:101:LEU:N	2.70	0.53
1:D:118:TYR:HE1	1:D:140:LEU:HG	1.73	0.53
1:C:79:PRO:HG2	1:D:78:ASP:OD1	2.08	0.53
1:A:106:SER:O	1:A:110:PHE:HD2	1.91	0.53
1:B:89:VAL:C	1:B:91:THR:H	2.12	0.53
1:D:27:VAL:HG12	1:D:31:LEU:HG	1.91	0.53
1:A:55:LEU:O	1:A:56:ARG:C	2.46	0.53
1:A:61:ALA:O	1:A:65:LEU:HG	2.09	0.53
1:C:122:PHE:C	1:C:124:VAL:N	2.62	0.53
1:C:35:ALA:O	1:C:39:ARG:HB2	2.08	0.53
1:D:21:SER:HB3	1:D:95:LEU:CD1	2.37	0.53
1:B:115:VAL:O	1:B:118:TYR:CB	2.57	0.52
1:C:139:ILE:CG2	1:C:140:LEU:H	2.21	0.52
1:D:106:SER:O	1:D:110:PHE:HD1	1.92	0.52
1:D:116:LEU:C	1:D:118:TYR:H	2.13	0.52
1:C:27:VAL:CG1	1:C:31:LEU:HD11	2.37	0.52
1:B:98:ARG:O	1:B:99:GLN:C	2.48	0.52
1:D:115:VAL:O	1:D:118:TYR:HB3	2.09	0.52
1:D:118:TYR:HB3	1:D:119:LEU:HD12	1.91	0.52
1:C:3:ILE:CD1	1:D:60:LEU:HD11	2.39	0.52
1:C:106:SER:O	1:C:110:PHE:HD1	1.91	0.52
1:B:5:PRO:HG2	1:B:6:TYR:CD2	2.44	0.52
1:C:6:TYR:OH	1:C:100:LEU:HB2	2.09	0.52
1:A:118:TYR:HB3	1:A:119:LEU:HD12	1.92	0.52
1:B:68:LEU:HG	1:B:69:ALA:N	2.24	0.52
1:B:88:TYR:O	1:B:92:ASN:N	2.42	0.52
1:B:31:LEU:O	1:B:32:ASP:C	2.48	0.52
1:C:3:ILE:O	1:C:3:ILE:HD12	2.10	0.52
1:C:77:GLU:HA	1:C:82:ARG:CZ	2.39	0.52
1:D:39:ARG:O	1:D:43:GLU:HG3	2.10	0.52
1:B:19:LEU:HD13	1:B:23:PHE:CD1	2.45	0.51
1:C:15:LEU:C	1:C:15:LEU:CD2	2.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:TYR:O	1:D:42:LEU:HD12	2.10	0.51
1:D:81:SER:C	1:D:83:ASP:H	2.07	0.51
1:D:89:VAL:C	1:D:91:THR:H	2.13	0.51
1:C:15:LEU:HD22	1:C:16:LEU:CD2	2.40	0.51
1:B:1:MET:HG2	1:B:3:ILE:HG23	1.92	0.51
1:C:97:PHE:O	1:C:101:LEU:HB2	2.10	0.51
1:A:85:VAL:HG23	1:A:86:VAL:N	2.26	0.51
1:C:86:VAL:HG12	1:C:90:ASN:HD22	1.76	0.51
1:D:1:MET:HG3	1:D:3:ILE:HG23	1.92	0.51
1:B:116:LEU:HD23	1:B:116:LEU:N	2.26	0.51
1:B:15:LEU:O	1:B:18:PHE:CD2	2.64	0.51
1:C:15:LEU:HD23	1:C:15:LEU:O	2.11	0.51
1:C:23:PHE:HD1	1:C:24:PHE:HA	1.75	0.51
1:A:118:TYR:CD2	1:A:140:LEU:HD21	2.46	0.51
1:A:38:TYR:O	1:A:41:ALA:HB3	2.11	0.51
1:B:68:LEU:HD13	1:A:88:TYR:HE2	1.75	0.51
1:A:65:LEU:O	1:A:68:LEU:HB3	2.11	0.51
1:B:37:LEU:HD12	1:B:37:LEU:O	2.11	0.51
1:A:53:THR:HA	1:A:56:ARG:HG3	1.93	0.50
1:B:109:THR:HB	1:B:110:PHE:CD2	2.46	0.50
1:D:93:VAL:C	1:D:95:LEU:H	2.14	0.50
1:A:16:LEU:C	1:A:18:PHE:N	2.65	0.50
1:B:54:ALA:O	1:B:55:LEU:C	2.49	0.50
1:D:6:TYR:C	1:D:8:GLU:H	2.14	0.50
1:A:100:LEU:HD23	1:A:101:LEU:CA	2.40	0.50
1:A:128:THR:O	1:A:129:PRO:C	2.50	0.50
1:C:84:LEU:O	1:C:84:LEU:HG	2.10	0.50
1:B:118:TYR:HE1	1:B:140:LEU:N	2.09	0.50
1:C:122:PHE:C	1:C:122:PHE:CD1	2.84	0.50
1:A:39:ARG:HG3	1:A:40:ASP:H	1.76	0.50
1:B:52:HIS:O	1:B:55:LEU:HB3	2.12	0.50
1:A:27:VAL:HG22	1:A:98:ARG:HG2	1.93	0.50
1:D:38:TYR:HB2	1:D:42:LEU:CD1	2.42	0.50
1:B:13:VAL:HG13	1:B:14:GLU:N	2.26	0.50
1:D:104:HIS:O	1:D:105:ILE:C	2.50	0.50
1:A:68:LEU:HG	1:A:69:ALA:N	2.27	0.49
1:D:85:VAL:CG2	1:D:86:VAL:HG23	2.42	0.49
1:A:55:LEU:HD11	1:A:104:HIS:CB	2.42	0.49
1:B:68:LEU:O	1:B:71:TRP:N	2.45	0.49
1:C:110:PHE:CD2	1:C:140:LEU:HB3	2.47	0.49
1:A:20:PRO:O	1:A:22:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLN:O	1:A:58:ALA:C	2.50	0.49
1:A:15:LEU:O	1:A:17:SER:N	2.46	0.49
1:B:30:LEU:HD23	1:B:105:ILE:HD12	1.93	0.49
1:B:25:PRO:O	1:B:30:LEU:CD1	2.61	0.49
1:C:43:GLU:HG2	1:D:3:ILE:HG22	1.94	0.49
1:D:138:PRO:O	1:D:139:ILE:HG13	2.12	0.49
1:B:137:ALA:HB1	1:B:138:PRO:HD2	1.93	0.49
1:A:56:ARG:HB2	1:A:57:GLN:HE21	1.76	0.49
1:A:103:PHE:CG	1:A:104:HIS:N	2.78	0.49
1:B:47:HIS:HB3	1:A:8:GLU:CG	2.42	0.49
1:D:100:LEU:O	1:D:101:LEU:C	2.51	0.49
1:D:116:LEU:O	1:D:118:TYR:N	2.46	0.49
1:A:68:LEU:O	1:A:71:TRP:HB3	2.12	0.49
1:C:119:LEU:O	1:C:123:GLY:N	2.39	0.49
1:B:112:ARG:O	1:B:115:VAL:N	2.38	0.48
1:B:38:TYR:O	1:B:39:ARG:C	2.51	0.48
1:C:25:PRO:HB2	1:C:30:LEU:CD1	2.43	0.48
1:D:4:ASP:OD1	1:D:6:TYR:HD2	1.95	0.48
1:A:6:TYR:CD1	1:A:6:TYR:N	2.80	0.48
1:B:65:LEU:HA	1:B:68:LEU:HB3	1.95	0.48
1:C:101:LEU:O	1:C:102:TRP:C	2.52	0.48
1:A:147:THR:O	1:A:148:VAL:O	2.31	0.48
1:B:55:LEU:O	1:B:58:ALA:N	2.46	0.48
1:B:18:PHE:O	1:B:20:PRO:HD3	2.13	0.48
1:C:116:LEU:HA	1:C:119:LEU:HD13	1.96	0.48
1:D:9:PHE:CD1	1:D:9:PHE:N	2.82	0.48
1:B:101:LEU:HD23	1:B:105:ILE:HD11	1.95	0.48
1:C:127:ARG:HD2	1:B:29:ASP:CB	2.43	0.48
1:B:62:TRP:HB2	1:B:97:PHE:CD2	2.49	0.48
1:C:6:TYR:C	1:C:8:GLU:H	2.16	0.48
1:A:15:LEU:C	1:A:15:LEU:CD2	2.82	0.48
1:B:24:PHE:HA	1:B:25:PRO:HD3	1.63	0.48
1:B:93:VAL:C	1:B:95:LEU:N	2.64	0.48
1:C:65:LEU:HA	1:C:68:LEU:HB3	1.94	0.48
1:A:4:ASP:OD1	1:A:6:TYR:HD1	1.95	0.48
1:D:100:LEU:O	1:D:103:PHE:HB3	2.14	0.48
1:C:3:ILE:CG2	1:D:43:GLU:HG2	2.30	0.48
1:C:87:SER:O	1:C:88:TYR:C	2.52	0.48
1:D:37:LEU:HG	1:D:38:TYR:CE1	2.49	0.48
1:A:128:THR:O	1:A:133:ARG:HG3	2.14	0.48
1:C:112:ARG:O	1:C:115:VAL:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG12	1:C:31:LEU:CD1	2.41	0.48
1:D:129:PRO:HA	1:D:130:PRO:HD3	1.78	0.48
1:A:44:SER:HA	1:A:45:PRO:HD3	1.70	0.47
1:B:39:ARG:NH2	1:A:1:MET:CB	2.76	0.47
1:B:134:PRO:O	1:B:136:ASN:N	2.47	0.47
1:C:30:LEU:H	1:C:30:LEU:HD12	1.79	0.47
1:D:109:THR:HB	1:D:110:PHE:CD1	2.48	0.47
1:A:62:TRP:HB2	1:A:97:PHE:CE2	2.49	0.47
1:B:20:PRO:O	1:B:23:PHE:HB3	2.13	0.47
1:C:85:VAL:HG23	1:C:86:VAL:N	2.30	0.47
1:C:102:TRP:O	1:C:103:PHE:C	2.53	0.47
1:A:15:LEU:HD23	1:A:16:LEU:N	2.28	0.47
1:C:16:LEU:CB	1:C:99:GLN:HE21	2.28	0.47
1:D:93:VAL:CG1	1:D:94:GLY:N	2.78	0.47
1:D:25:PRO:O	1:D:30:LEU:HD13	2.15	0.47
1:B:100:LEU:O	1:B:101:LEU:C	2.52	0.47
1:C:122:PHE:C	1:C:124:VAL:H	2.18	0.47
1:C:50:PRO:O	1:C:51:HIS:C	2.53	0.47
1:A:34:ALA:O	1:A:37:LEU:N	2.48	0.47
1:B:42:LEU:O	1:B:44:SER:N	2.47	0.47
1:C:123:GLY:O	1:C:127:ARG:HB2	2.15	0.47
1:C:118:TYR:OH	1:C:139:ILE:HG12	2.14	0.47
1:C:144:PRO:O	1:C:145:GLU:HG2	2.14	0.47
1:D:44:SER:HA	1:D:45:PRO:HD3	1.69	0.47
1:A:139:ILE:CG2	1:A:140:LEU:N	2.46	0.46
1:B:47:HIS:HB3	1:A:8:GLU:HG3	1.97	0.46
1:D:116:LEU:C	1:D:118:TYR:N	2.68	0.46
1:B:126:ILE:C	1:B:128:THR:H	2.19	0.46
1:D:62:TRP:HA	1:D:65:LEU:HD12	1.97	0.46
1:A:88:TYR:O	1:A:92:ASN:HB2	2.14	0.46
1:D:119:LEU:N	1:D:119:LEU:CD1	2.67	0.46
1:B:13:VAL:O	1:B:16:LEU:N	2.48	0.46
1:C:34:ALA:O	1:C:37:LEU:N	2.47	0.46
1:A:12:THR:HG23	1:A:15:LEU:N	2.31	0.46
1:B:23:PHE:O	1:B:23:PHE:CD2	2.67	0.46
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.47	0.46
1:B:47:HIS:HB3	1:A:8:GLU:CD	2.36	0.46
1:A:116:LEU:HA	1:A:119:LEU:HD13	1.98	0.46
1:B:3:ILE:HD12	1:B:3:ILE:O	2.16	0.46
1:C:54:ALA:O	1:C:55:LEU:C	2.53	0.46
1:D:6:TYR:O	1:D:8:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:VAL:O	1:D:86:VAL:HG12	2.16	0.46
1:A:134:PRO:O	1:A:136:ASN:N	2.49	0.46
1:A:35:ALA:O	1:A:39:ARG:HB3	2.16	0.46
1:B:116:LEU:HA	1:B:119:LEU:HD13	1.98	0.46
1:B:119:LEU:O	1:B:120:VAL:C	2.55	0.46
1:C:111:GLY:O	1:C:115:VAL:HG23	2.16	0.46
1:C:3:ILE:HD11	1:D:60:LEU:HD11	1.97	0.46
1:D:38:TYR:HB3	1:D:41:ALA:HB3	1.98	0.46
1:D:81:SER:C	1:D:83:ASP:N	2.66	0.46
1:A:115:VAL:O	1:A:119:LEU:CD1	2.64	0.45
1:A:6:TYR:O	1:A:9:PHE:N	2.48	0.45
1:B:93:VAL:O	1:B:94:GLY:C	2.53	0.45
1:C:118:TYR:O	1:C:119:LEU:C	2.54	0.45
1:C:49:SER:HB2	1:C:50:PRO:HD2	1.98	0.45
1:C:59:ILE:O	1:C:63:GLY:N	2.40	0.45
1:D:30:LEU:CD2	1:D:101:LEU:HD22	2.46	0.45
1:A:19:LEU:HA	1:A:20:PRO:HD3	1.89	0.45
1:C:115:VAL:O	1:C:118:TYR:CB	2.64	0.45
1:D:55:LEU:O	1:D:56:ARG:C	2.53	0.45
1:D:115:VAL:O	1:D:118:TYR:N	2.42	0.45
1:B:100:LEU:C	1:B:100:LEU:CD2	2.84	0.45
1:C:8:GLU:OE2	1:D:53:THR:HG23	2.16	0.45
1:A:88:TYR:O	1:A:88:TYR:CG	2.70	0.45
1:C:35:ALA:HB3	1:D:1:MET:HE1	1.99	0.45
1:D:25:PRO:HB2	1:D:30:LEU:CD1	2.46	0.45
1:D:55:LEU:O	1:D:58:ALA:HB3	2.16	0.45
1:D:89:VAL:O	1:D:91:THR:N	2.49	0.45
1:A:110:PHE:HB3	1:A:114:THR:HG21	1.99	0.45
1:D:25:PRO:HB2	1:D:30:LEU:HD12	1.98	0.45
1:D:50:PRO:O	1:D:51:HIS:C	2.55	0.45
1:D:77:GLU:HA	1:D:82:ARG:CD	2.44	0.45
1:A:115:VAL:O	1:A:118:TYR:HB3	2.16	0.45
1:A:3:ILE:O	1:A:3:ILE:CG1	2.65	0.45
1:C:18:PHE:HE2	1:C:123:GLY:C	2.19	0.45
1:D:122:PHE:C	1:D:124:VAL:N	2.69	0.45
1:B:118:TYR:O	1:B:119:LEU:C	2.54	0.45
1:A:103:PHE:O	1:A:104:HIS:C	2.55	0.45
1:B:5:PRO:HG2	1:B:6:TYR:CE2	2.52	0.45
1:B:15:LEU:HD22	1:B:16:LEU:CD2	2.45	0.45
1:C:110:PHE:CD1	1:C:110:PHE:N	2.84	0.45
1:C:42:LEU:C	1:C:44:SER:N	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:HIS:O	1:C:53:THR:C	2.55	0.45
1:A:55:LEU:O	1:A:58:ALA:HB3	2.16	0.44
1:B:111:GLY:O	1:B:115:VAL:HG23	2.17	0.44
1:B:30:LEU:O	1:B:33:THR:HB	2.17	0.44
1:B:65:LEU:HD23	1:B:65:LEU:N	2.31	0.44
1:C:23:PHE:HD1	1:C:24:PHE:CA	2.30	0.44
1:C:86:VAL:HG12	1:C:90:ASN:ND2	2.31	0.44
1:D:89:VAL:HA	1:D:93:VAL:CG1	2.41	0.44
1:A:107:ALA:C	1:A:109:THR:N	2.71	0.44
1:A:3:ILE:O	1:A:3:ILE:HG13	2.17	0.44
1:B:15:LEU:HD23	1:B:15:LEU:C	2.38	0.44
1:D:107:ALA:HB2	1:D:115:VAL:HG21	1.99	0.44
1:B:107:ALA:C	1:B:109:THR:N	2.69	0.44
1:C:100:LEU:CD2	1:C:100:LEU:C	2.86	0.44
1:A:100:LEU:C	1:A:100:LEU:HD23	2.37	0.44
1:A:27:VAL:O	1:A:28:ARG:C	2.55	0.44
1:A:27:VAL:O	1:A:30:LEU:N	2.50	0.44
1:A:31:LEU:C	1:A:33:THR:N	2.70	0.44
1:D:13:VAL:O	1:D:16:LEU:N	2.43	0.44
1:D:76:LEU:O	1:D:82:ARG:HD3	2.18	0.44
1:A:25:PRO:O	1:A:30:LEU:CD1	2.66	0.44
1:A:85:VAL:CG2	1:A:86:VAL:N	2.79	0.44
1:B:134:PRO:C	1:B:136:ASN:N	2.71	0.44
1:B:25:PRO:O	1:B:26:SER:C	2.56	0.44
1:B:44:SER:HA	1:B:45:PRO:HD3	1.69	0.44
1:B:85:VAL:CG2	1:B:86:VAL:H	2.29	0.44
1:D:27:VAL:HG12	1:D:31:LEU:CG	2.46	0.44
1:D:51:HIS:O	1:D:54:ALA:HB3	2.17	0.44
1:B:119:LEU:HD12	1:B:119:LEU:N	2.12	0.44
1:B:20:PRO:HG3	1:B:126:ILE:HD12	2.00	0.44
1:C:119:LEU:O	1:C:120:VAL:C	2.56	0.44
1:C:95:LEU:HA	1:C:98:ARG:HG2	2.00	0.44
1:B:116:LEU:HD23	1:B:116:LEU:H	1.81	0.44
1:C:88:TYR:CE2	1:D:68:LEU:HD13	2.52	0.44
1:A:57:GLN:NE2	1:A:57:GLN:H	2.15	0.44
1:A:142:THR:O	1:A:144:PRO:CD	2.62	0.44
1:A:13:VAL:CG1	1:A:14:GLU:N	2.80	0.44
1:C:115:VAL:O	1:C:118:TYR:HB3	2.17	0.44
1:C:13:VAL:C	1:C:15:LEU:N	2.69	0.44
1:C:143:LEU:CB	1:C:144:PRO:CD	2.96	0.44
1:C:13:VAL:O	1:C:15:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ASP:HA	1:D:5:PRO:HD3	1.65	0.44
1:D:100:LEU:HD23	1:D:101:LEU:CA	2.48	0.43
1:D:52:HIS:O	1:D:56:ARG:HG3	2.17	0.43
1:A:115:VAL:O	1:A:116:LEU:C	2.57	0.43
1:A:57:GLN:O	1:A:60:LEU:N	2.51	0.43
1:B:6:TYR:HB2	1:B:12:THR:HA	2.00	0.43
1:D:13:VAL:O	1:D:15:LEU:N	2.51	0.43
1:D:77:GLU:O	1:D:77:GLU:HG2	2.18	0.43
1:C:55:LEU:O	1:C:56:ARG:C	2.55	0.43
1:A:129:PRO:HA	1:A:130:PRO:HD3	1.66	0.43
1:A:142:THR:CG2	1:A:143:LEU:N	2.82	0.43
1:A:62:TRP:C	1:A:64:ASP:H	2.21	0.43
1:C:107:ALA:O	1:C:109:THR:N	2.50	0.43
1:D:54:ALA:O	1:D:55:LEU:C	2.56	0.43
1:B:134:PRO:C	1:B:136:ASN:H	2.21	0.43
1:C:35:ALA:HB1	1:D:1:MET:HE1	2.01	0.43
1:D:19:LEU:HA	1:D:20:PRO:HD3	1.86	0.43
1:B:131:ALA:C	1:B:132:TYR:HD2	2.22	0.43
1:C:86:VAL:O	1:C:89:VAL:HB	2.18	0.43
1:A:33:THR:O	1:A:34:ALA:C	2.57	0.43
1:A:120:VAL:HB	1:A:121:SER:H	1.44	0.43
1:A:31:LEU:O	1:A:33:THR:N	2.52	0.43
1:A:1:MET:HG3	1:A:3:ILE:CG2	2.48	0.43
1:A:30:LEU:N	1:A:30:LEU:HD12	2.34	0.43
1:B:47:HIS:O	1:B:48:ALA:C	2.58	0.43
1:D:51:HIS:O	1:D:55:LEU:HD13	2.18	0.43
1:D:27:VAL:HG12	1:D:31:LEU:HD11	2.00	0.42
1:A:97:PHE:O	1:A:101:LEU:HB2	2.20	0.42
1:A:110:PHE:CE1	1:A:140:LEU:O	2.72	0.42
1:B:109:THR:HB	1:B:110:PHE:CE2	2.54	0.42
1:C:119:LEU:CD1	1:C:119:LEU:N	2.77	0.42
1:C:3:ILE:HD12	1:D:60:LEU:HD11	2.02	0.42
1:D:15:LEU:HD23	1:D:16:LEU:HD21	2.00	0.42
1:A:115:VAL:HG12	1:A:119:LEU:HD11	2.01	0.42
1:B:13:VAL:O	1:B:15:LEU:N	2.52	0.42
1:C:19:LEU:HA	1:C:20:PRO:HD3	1.79	0.42
1:C:67:THR:CG2	1:C:67:THR:O	2.68	0.42
1:D:24:PHE:HA	1:D:25:PRO:HD3	1.82	0.42
1:D:38:TYR:HB2	1:D:42:LEU:HD12	2.01	0.42
1:A:123:GLY:C	1:A:127:ARG:HE	2.23	0.42
1:B:95:LEU:O	1:B:97:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PRO:C	1:C:145:GLU:CG	2.88	0.42
1:C:8:GLU:CD	1:D:47:HIS:HB3	2.40	0.42
1:A:31:LEU:O	1:A:32:ASP:C	2.58	0.42
1:B:51:HIS:O	1:B:52:HIS:C	2.58	0.42
1:B:6:TYR:C	1:B:8:GLU:N	2.71	0.42
1:C:119:LEU:O	1:C:120:VAL:O	2.38	0.42
1:C:38:TYR:HB2	1:C:42:LEU:HD11	2.00	0.42
1:A:4:ASP:OD1	1:A:6:TYR:CD1	2.72	0.42
1:B:34:ALA:O	1:B:37:LEU:N	2.36	0.42
1:B:3:ILE:CG1	1:B:3:ILE:O	2.67	0.42
1:A:115:VAL:O	1:A:119:LEU:HD12	2.20	0.42
1:A:13:VAL:HG13	1:A:14:GLU:H	1.84	0.42
1:A:24:PHE:HA	1:A:25:PRO:HD3	1.72	0.42
1:D:19:LEU:HG	1:D:19:LEU:H	1.40	0.42
1:A:15:LEU:HD21	1:A:119:LEU:HD23	2.01	0.42
1:A:4:ASP:HA	1:A:5:PRO:HD3	1.78	0.42
1:C:18:PHE:CE1	1:B:33:THR:HA	2.33	0.42
1:D:20:PRO:O	1:D:23:PHE:HB3	2.19	0.42
1:B:105:ILE:HG22	1:B:106:SER:N	2.34	0.42
1:B:55:LEU:O	1:B:58:ALA:HB3	2.20	0.42
1:B:104:HIS:O	1:B:107:ALA:HB3	2.20	0.41
1:C:34:ALA:O	1:C:37:LEU:HB3	2.20	0.41
1:B:26:SER:O	1:B:29:ASP:HB2	2.20	0.41
1:D:4:ASP:OD1	1:D:5:PRO:HD2	2.20	0.41
1:B:95:LEU:O	1:B:96:LYS:C	2.56	0.41
1:C:137:ALA:HA	1:C:138:PRO:HD3	1.94	0.41
1:D:37:LEU:HG	1:D:38:TYR:CZ	2.55	0.41
1:D:79:PRO:HG2	1:D:81:SER:OG	2.20	0.41
1:B:101:LEU:O	1:B:102:TRP:C	2.58	0.41
1:B:122:PHE:CD2	1:B:122:PHE:C	2.93	0.41
1:B:50:PRO:HG2	1:A:47:HIS:HD2	1.85	0.41
1:B:89:VAL:C	1:B:91:THR:N	2.73	0.41
1:D:62:TRP:HB2	1:D:97:PHE:CE1	2.55	0.41
1:A:16:LEU:C	1:A:18:PHE:H	2.24	0.41
1:C:140:LEU:N	1:C:140:LEU:HD23	2.35	0.41
1:C:143:LEU:HB2	1:C:144:PRO:CD	2.50	0.41
1:C:27:VAL:O	1:C:28:ARG:C	2.58	0.41
1:A:115:VAL:O	1:A:118:TYR:CB	2.69	0.41
1:A:118:TYR:HD1	1:A:119:LEU:N	2.18	0.41
1:B:100:LEU:HD22	1:B:101:LEU:N	2.35	0.41
1:B:15:LEU:CD2	1:B:16:LEU:HD23	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ALA:C	1:C:109:THR:N	2.73	0.41
1:A:100:LEU:HD23	1:A:101:LEU:HA	2.03	0.41
1:A:24:PHE:CD2	1:A:99:GLN:HA	2.56	0.41
1:B:62:TRP:C	1:B:64:ASP:N	2.73	0.41
1:C:106:SER:O	1:C:107:ALA:C	2.59	0.41
1:C:6:TYR:O	1:C:7:LYS:C	2.59	0.41
1:D:119:LEU:O	1:D:120:VAL:C	2.59	0.41
1:B:3:ILE:HG13	1:B:3:ILE:O	2.21	0.41
1:D:104:HIS:O	1:D:106:SER:N	2.54	0.41
1:D:98:ARG:O	1:D:99:GLN:O	2.39	0.41
1:A:15:LEU:O	1:A:16:LEU:C	2.59	0.41
1:A:98:ARG:O	1:A:99:GLN:C	2.59	0.41
1:B:19:LEU:HD13	1:B:23:PHE:CE1	2.55	0.41
1:B:28:ARG:O	1:B:32:ASP:OD2	2.39	0.41
1:C:115:VAL:O	1:C:116:LEU:C	2.57	0.41
1:C:87:SER:O	1:C:89:VAL:N	2.54	0.41
1:D:126:ILE:HG23	1:D:127:ARG:HG2	2.02	0.41
1:A:118:TYR:CD2	1:A:140:LEU:CD2	3.04	0.41
1:B:126:ILE:HG23	1:B:127:ARG:N	2.35	0.41
1:C:13:VAL:O	1:C:16:LEU:N	2.54	0.41
1:C:93:VAL:HG13	1:C:94:GLY:N	2.35	0.41
1:D:116:LEU:HA	1:D:119:LEU:HD13	2.02	0.41
1:D:25:PRO:O	1:D:30:LEU:CD1	2.69	0.41
1:A:12:THR:HG23	1:A:15:LEU:CB	2.50	0.41
1:A:30:LEU:O	1:A:33:THR:HB	2.21	0.41
1:A:57:GLN:HB2	1:A:58:ALA:H	1.63	0.41
1:B:134:PRO:HA	1:B:135:PRO:HD3	1.96	0.41
1:D:38:TYR:HB2	1:D:42:LEU:HD11	2.03	0.41
1:A:37:LEU:HD12	1:A:37:LEU:O	2.21	0.40
1:C:103:PHE:CG	1:C:104:HIS:N	2.87	0.40
1:C:116:LEU:O	1:C:119:LEU:HD13	2.20	0.40
1:C:143:LEU:CB	1:C:144:PRO:HD3	2.52	0.40
1:C:55:LEU:HD23	1:C:56:ARG:CA	2.51	0.40
1:D:124:VAL:O	1:D:125:TRP:C	2.60	0.40
1:D:27:VAL:O	1:D:28:ARG:C	2.59	0.40
1:D:76:LEU:O	1:D:82:ARG:CD	2.69	0.40
1:A:127:ARG:H	1:A:127:ARG:HG2	1.68	0.40
1:C:52:HIS:O	1:C:56:ARG:HG3	2.22	0.40
1:A:104:HIS:O	1:A:105:ILE:C	2.59	0.40
1:A:127:ARG:O	1:A:127:ARG:HG3	2.21	0.40
1:A:15:LEU:HD22	1:A:16:LEU:N	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.93	0.40
1:B:128:THR:HA	1:B:129:PRO:HD2	1.61	0.40
1:B:52:HIS:HB3	1:B:56:ARG:NH1	2.37	0.40
1:D:27:VAL:HG12	1:D:31:LEU:CD1	2.51	0.40
1:A:2:ASP:C	1:A:3:ILE:HG23	2.42	0.40
1:A:62:TRP:O	1:A:65:LEU:HB2	2.22	0.40
1:B:46:GLU:C	1:B:48:ALA:H	2.24	0.40
1:B:62:TRP:HA	1:B:65:LEU:HG	2.03	0.40
1:C:57:GLN:O	1:C:58:ALA:C	2.59	0.40
1:D:141:SER:C	1:D:143:LEU:N	2.73	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	146/150 (97%)	78 (53%)	41 (28%)	27 (18%)	0	2
1	B	145/150 (97%)	86 (59%)	36 (25%)	23 (16%)	0	4
1	C	145/150 (97%)	76 (52%)	37 (26%)	32 (22%)	0	1
1	D	144/150 (96%)	80 (56%)	40 (28%)	24 (17%)	0	4
All	All	580/600 (97%)	320 (55%)	154 (27%)	106 (18%)	0	3

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	ALA
1	C	39	ARG
1	C	48	ALA
1	C	54	ALA
1	C	78	ASP

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Mol	Chain	Res	Type
1	C	79	PRO
1	C	120	VAL
1	C	130	PRO
1	D	48	ALA
1	D	78	ASP
1	D	99	GLN
1	D	103	PHE
1	D	127	ARG
1	D	143	LEU
1	B	34	ALA
1	B	56	ARG
1	B	89	VAL
1	B	101	LEU
1	B	105	ILE
1	B	120	VAL
1	A	34	ALA
1	A	48	ALA
1	A	56	ARG
1	A	99	GLN
1	A	103	PHE
1	A	119	LEU
1	A	120	VAL
1	C	7	LYS
1	C	52	HIS
1	C	89	VAL
1	C	99	GLN
1	C	103	PHE
1	C	105	ILE
1	C	118	TYR
1	C	123	GLY
1	C	142	THR
1	D	55	LEU
1	D	89	VAL
1	D	90	ASN
1	D	104	HIS
1	D	105	ILE
1	D	111	GLY
1	B	2	ASP
1	B	39	ARG
1	B	53	THR
1	B	55	LEU
1	B	90	ASN

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Mol	Chain	Res	Type
1	B	100	LEU
1	B	103	PHE
1	A	14	GLU
1	A	16	LEU
1	A	17	SER
1	A	18	PHE
1	A	90	ASN
1	A	101	LEU
1	A	104	HIS
1	A	105	ILE
1	C	35	ALA
1	C	53	THR
1	C	55	LEU
1	C	88	TYR
1	C	104	HIS
1	C	108	LEU
1	C	134	PRO
1	D	18	PHE
1	D	37	LEU
1	D	54	ALA
1	D	117	GLU
1	B	129	PRO
1	A	39	ARG
1	A	55	LEU
1	A	57	GLN
1	A	58	ALA
1	A	100	LEU
1	A	102	TRP
1	A	108	LEU
1	A	129	PRO
1	C	84	LEU
1	C	119	LEU
1	D	34	ALA
1	D	69	ALA
1	D	100	LEU
1	D	130	PRO
1	B	35	ALA
1	B	48	ALA
1	A	21	SER
1	A	85	VAL
1	C	14	GLU
1	C	87	SER

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Mol	Chain	Res	Type
1	D	56	ARG
1	D	123	GLY
1	B	33	THR
1	B	102	TRP
1	A	143	LEU
1	C	27	VAL
1	C	146	THR
1	B	43	GLU
1	B	54	ALA
1	B	108	LEU
1	B	127	ARG
1	B	130	PRO
1	C	129	PRO
1	D	120	VAL
1	C	143	LEU
1	D	79	PRO
1	A	135	PRO

### 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	124/130 (95%)	118 (95%)	6 (5%)	30	65
1	B	127/130 (98%)	117 (92%)	10 (8%)	14	50
1	C	127/130 (98%)	119 (94%)	8 (6%)	21	57
1	D	126/130 (97%)	116 (92%)	10 (8%)	14	50
All	All	504/520 (97%)	470 (93%)	34 (7%)	19	56

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	PHE
1	C	24	PHE
1	C	47	HIS
1	C	88	TYR

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Mol	Chain	Res	Type
1	C	100	LEU
1	C	101	LEU
1	C	119	LEU
1	C	144	PRO
1	D	19	LEU
1	D	23	PHE
1	D	88	TYR
1	D	101	LEU
1	D	108	LEU
1	D	109	THR
1	D	119	LEU
1	D	129	PRO
1	D	142	THR
1	D	144	PRO
1	B	1	MET
1	B	12	THR
1	B	19	LEU
1	B	23	PHE
1	B	47	HIS
1	B	55	LEU
1	B	68	LEU
1	B	101	LEU
1	B	108	LEU
1	B	116	LEU
1	A	23	PHE
1	A	24	PHE
1	A	47	HIS
1	A	49	SER
1	A	101	LEU
1	A	129	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	ASN
1	C	99	GLN
1	B	90	ASN
1	A	57	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, 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	148/150 (98%)	-0.46	1 (0%) 87 82	44, 95, 160, 196	0
1	B	147/150 (98%)	-0.46	4 (2%) 55 44	43, 94, 159, 200	0
1	C	147/150 (98%)	-0.27	5 (3%) 46 36	35, 105, 176, 200	0
1	D	146/150 (97%)	-0.27	1 (0%) 87 82	40, 106, 171, 194	0
All	All	588/600 (98%)	-0.37	11 (1%) 67 58	35, 100, 172, 200	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	THR	5.1
1	C	145	GLU	3.9
1	B	146	THR	3.7
1	C	146	THR	3.5
1	B	145	GLU	2.7
1	D	80	ALA	2.5
1	C	84	LEU	2.4
1	A	146	THR	2.4
1	B	144	PRO	2.3
1	C	147	THR	2.2
1	C	91	THR	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.