



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 07:05 AM EDT

PDB ID : 1JQU
Title : Are Carboxy Terminii of Helices Coded by the Local Sequence or by Tertiary Structure Contacts
Authors : Sagermann, M.; Martensson, L.-G.; Baase, W.A.; Matthews, B.W.
Deposited on : 2001-08-08
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

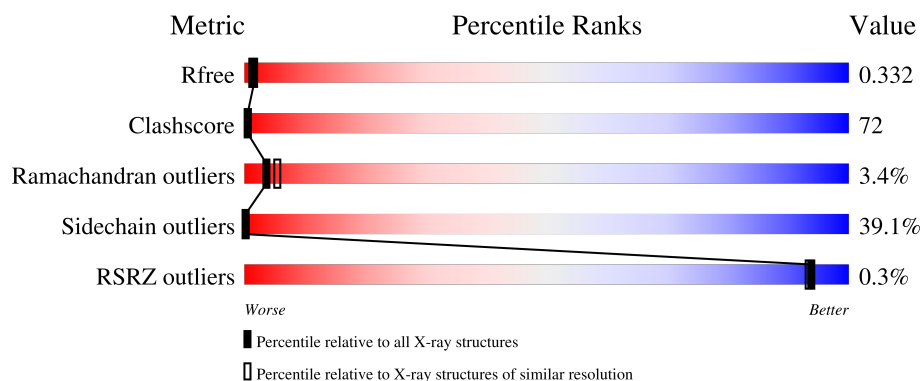
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	164	<div> <div>%</div> <div> <div></div> <div>31%</div> <div>52%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	164	<div> <div>25%</div> <div>44%</div> <div>29%</div> <div>.</div> </div>
1	C	164	<div> <div>21%</div> <div>48%</div> <div>28%</div> <div>.</div> </div>
1	D	164	<div> <div>%</div> <div>16%</div> <div>49%</div> <div>30%</div> <div>5%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5241 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 Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			
1	B	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			
1	C	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			
1	D	164	Total	C	N	O	S	0	0	0
			1303	819	237	242	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	THR	CIS	engineered mutation	UNP P00720
A	97	ALA	CIS	engineered mutation	UNP P00720
A	158	LEU	TRP	engineered mutation	UNP P00720
B	54	THR	CIS	engineered mutation	UNP P00720
B	97	ALA	CIS	engineered mutation	UNP P00720
B	158	LEU	TRP	engineered mutation	UNP P00720
C	54	THR	CIS	engineered mutation	UNP P00720
C	97	ALA	CIS	engineered mutation	UNP P00720
C	158	LEU	TRP	engineered mutation	UNP P00720
D	54	THR	CIS	engineered mutation	UNP P00720
D	97	ALA	CIS	engineered mutation	UNP P00720
D	158	LEU	TRP	engineered mutation	UNP P00720

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	9	Total	O	0	0
			9	9		

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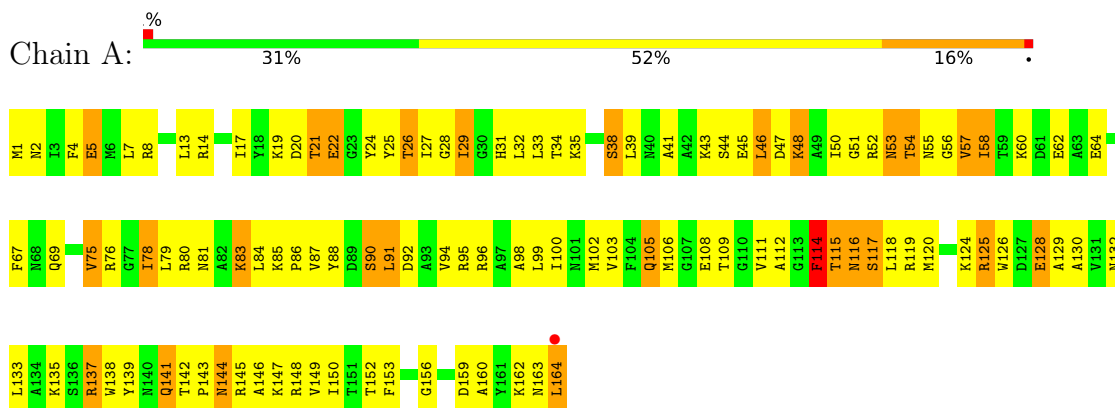
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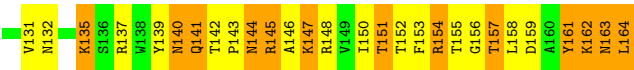
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	13	Total	O	0	0
			13	13		
2	D	2	Total	O	0	0
			2	2		

3 Residue-property plots

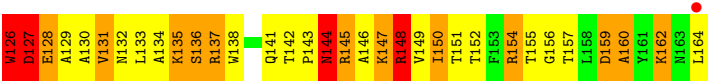
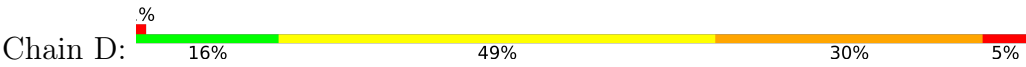
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Lysozyme





● Molecule 1: Lysozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.30Å 77.20Å 138.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.60 34.92 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.60) 78.8 (34.92-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 2.48Å)	Xtriage
Refinement program	TNT, CNS	Depositor
R, R_{free}	0.229 , 0.316 0.212 , 0.332	Depositor DCC
R_{free} test set	2228 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 127.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5241	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.59	0/1321	0.61	1/1777 (0.1%)
1	B	0.54	0/1321	0.85	1/1777 (0.1%)
1	C	1.22	14/1321 (1.1%)	1.25	18/1777 (1.0%)
1	D	1.28	10/1321 (0.8%)	1.57	19/1777 (1.1%)
All	All	0.97	24/5284 (0.5%)	1.13	39/7108 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	7
1	D	0	5
All	All	0	12

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	PHE	CB-CG	-23.47	1.11	1.51
1	D	127	ASP	CB-CG	21.39	1.96	1.51
1	D	50	ILE	CB-CG1	17.73	2.03	1.54
1	D	50	ILE	C-N	-16.20	1.03	1.33
1	D	124	LYS	CB-CG	14.27	1.91	1.52
1	D	125	ARG	CB-CG	12.04	1.85	1.52
1	C	114	PHE	CB-CG	-11.77	1.31	1.51
1	C	31	HIS	CB-CG	11.64	1.71	1.50
1	C	34	THR	CB-CG2	10.82	1.88	1.52
1	D	126	TRP	CB-CG	-9.24	1.33	1.50
1	C	2	ASN	CB-CG	8.41	1.70	1.51
1	C	34	THR	CB-OG1	8.39	1.60	1.43
1	C	32	LEU	CB-CG	8.05	1.75	1.52
1	D	48	LYS	C-N	7.97	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	GLU	CB-CG	6.90	1.65	1.52
1	D	126	TRP	C-N	-6.90	1.18	1.34
1	C	11	GLU	CB-CG	-6.74	1.39	1.52
1	D	50	ILE	CB-CG2	6.69	1.73	1.52
1	C	4	PHE	CA-CB	6.57	1.68	1.53
1	D	127	ASP	N-CA	6.06	1.58	1.46
1	C	10	ASP	C-N	-5.32	1.21	1.34
1	C	34	THR	C-N	-5.21	1.22	1.34
1	C	30	GLY	C-N	-5.17	1.22	1.34
1	C	113	GLY	C-N	-5.08	1.22	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	TRP	O-C-N	-26.84	79.76	122.70
1	B	36	SER	C-N-CD	-24.21	67.34	120.60
1	D	50	ILE	O-C-N	-24.16	82.12	123.20
1	C	114	PHE	CB-CG-CD2	-20.01	106.79	120.80
1	D	50	ILE	C-N-CA	19.23	162.69	122.30
1	D	50	ILE	CA-C-N	16.72	149.64	116.20
1	D	126	TRP	N-CA-CB	14.27	136.28	110.60
1	D	126	TRP	CB-CA-C	-13.12	84.16	110.40
1	C	34	THR	CA-CB-CG2	-13.03	94.16	112.40
1	C	114	PHE	CA-CB-CG	12.65	144.25	113.90
1	D	126	TRP	CA-C-N	12.41	144.49	117.20
1	D	50	ILE	CG1-CB-CG2	-12.13	84.72	111.40
1	D	125	ARG	CA-CB-CG	-11.81	87.42	113.40
1	C	32	LEU	CB-CG-CD1	11.68	130.85	111.00
1	D	126	TRP	C-N-CA	11.56	150.60	121.70
1	D	52	ARG	O-C-N	-11.24	104.71	122.70
1	C	114	PHE	CB-CG-CD1	9.69	127.59	120.80
1	C	34	THR	OG1-CB-CG2	-9.56	88.02	110.00
1	C	32	LEU	CA-CB-CG	-9.24	94.05	115.30
1	D	50	ILE	CA-CB-CG1	-9.05	93.81	111.00
1	C	1	MET	O-C-N	-8.96	108.36	122.70
1	C	4	PHE	CB-CG-CD2	8.87	127.01	120.80
1	C	34	THR	O-C-N	-8.75	108.69	122.70
1	C	4	PHE	CB-CG-CD1	-8.66	114.74	120.80
1	C	2	ASN	CA-CB-CG	-8.40	94.91	113.40
1	D	125	ARG	O-C-N	7.32	134.41	122.70
1	A	142	THR	C-N-CD	-7.31	104.52	120.60
1	D	126	TRP	CB-CG-CD2	-7.08	117.40	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	LYS	O-C-N	7.04	133.97	122.70
1	C	1	MET	C-N-CA	6.67	138.37	121.70
1	C	115	THR	CA-CB-CG2	-6.43	103.40	112.40
1	D	127	ASP	CA-CB-CG	-6.20	99.76	113.40
1	C	1	MET	CA-C-N	6.13	130.69	117.20
1	D	124	LYS	CA-CB-CG	-6.05	100.09	113.40
1	D	126	TRP	CA-C-O	5.79	132.26	120.10
1	C	5	GLU	CA-CB-CG	-5.60	101.07	113.40
1	C	2	ASN	CB-CG-OD1	-5.51	110.58	121.60
1	C	32	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	D	50	ILE	CA-CB-CG2	-5.16	100.58	110.90

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	MET	Peptide,Mainchain
1	C	114	PHE	Sidechain
1	C	2	ASN	Mainchain
1	C	30	GLY	Mainchain
1	C	33	LEU	Mainchain
1	C	34	THR	Mainchain
1	D	126	TRP	Peptide,Mainchain
1	D	50	ILE	Peptide,Mainchain
1	D	52	ARG	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1303	0	1337	139	0
1	B	1303	0	1337	205	0
1	C	1303	0	1333	200	0
1	D	1303	0	1335	240	0
2	A	5	0	0	4	0
2	B	9	0	0	6	0
2	C	13	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	2	0
All	All	5241	0	5342	762	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 72.

All (762) 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:C:32:LEU:CB	1:C:32:LEU:CG	1.75	1.57
1:D:125:ARG:CG	1:D:125:ARG:CB	1.85	1.52
1:C:34:THR:CB	1:C:34:THR:CG2	1.88	1.50
1:D:124:LYS:CG	1:D:124:LYS:CB	1.91	1.48
1:D:50:ILE:CB	1:D:50:ILE:CG1	2.03	1.34
1:D:127:ASP:CB	1:D:127:ASP:CG	1.96	1.32
1:B:52:ARG:CZ	1:B:54:THR:HG22	1.62	1.28
1:D:125:ARG:CB	1:D:128:GLU:HG3	1.68	1.24
1:B:52:ARG:NE	1:B:54:THR:HG22	1.53	1.22
1:D:125:ARG:HB3	1:D:128:GLU:CG	1.72	1.17
1:C:114:PHE:O	1:C:118:LEU:HD12	1.46	1.15
1:A:52:ARG:CZ	1:A:54:THR:HG23	1.80	1.12
1:C:58:ILE:HD12	1:C:63:ALA:HB2	1.27	1.11
1:B:50:ILE:HD12	1:B:54:THR:HG21	1.32	1.10
1:B:52:ARG:CZ	1:B:54:THR:CG2	2.29	1.09
1:C:50:ILE:HG13	1:C:62:GLU:HG2	1.36	1.08
1:D:52:ARG:O	1:D:52:ARG:HG2	1.34	1.08
1:C:34:THR:HG23	1:C:34:THR:O	1.56	1.05
1:D:2:ASN:HD21	1:D:4:PHE:HB3	1.17	1.04
1:B:50:ILE:HD12	1:B:54:THR:CG2	1.89	1.02
1:C:157:THR:HG23	1:C:159:ASP:H	1.24	1.02
1:D:125:ARG:CG	1:D:125:ARG:CA	2.36	1.02
1:D:78:ILE:HG23	1:D:84:LEU:HB3	1.42	1.00
1:B:59:THR:HG22	1:B:62:GLU:H	1.23	1.00
1:A:144:ASN:HD21	1:B:162:LYS:NZ	1.61	0.99
1:C:32:LEU:CG	1:C:32:LEU:CA	2.41	0.98
1:C:114:PHE:O	1:C:118:LEU:CD1	2.10	0.97
1:A:159:ASP:HA	1:A:162:LYS:HG3	1.45	0.97
1:B:126:TRP:HB3	1:B:154:ARG:HA	1.47	0.95
1:A:148:ARG:HH11	1:A:164:LEU:HD13	1.29	0.95
1:D:6:MET:HE1	1:D:101:ASN:HB2	1.49	0.94
1:C:151:THR:HA	1:C:154:ARG:NH1	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ARG:HD2	1:B:18:TYR:CE2	2.05	0.92
1:C:101:ASN:HD21	1:C:145:ARG:HH21	1.11	0.91
1:C:154:ARG:HH11	1:C:154:ARG:HB3	1.36	0.90
1:B:59:THR:HG23	1:B:61:ASP:H	1.35	0.90
1:C:50:ILE:CG1	1:C:62:GLU:HG2	2.02	0.90
1:D:52:ARG:O	1:D:54:THR:N	2.05	0.90
1:A:83:LYS:NZ	1:A:115:THR:HG23	1.87	0.89
1:B:52:ARG:CG	1:B:54:THR:CG2	2.49	0.89
1:A:52:ARG:CZ	1:A:54:THR:CG2	2.50	0.88
1:C:34:THR:CG2	1:C:34:THR:CA	2.51	0.88
1:B:79:LEU:HA	1:B:85:LYS:HG2	1.55	0.88
1:B:47:ASP:HA	1:B:50:ILE:HG22	1.54	0.87
1:C:144:ASN:HA	1:C:147:LYS:HE2	1.57	0.87
1:B:58:ILE:HG13	1:B:62:GLU:HB3	1.55	0.86
1:A:52:ARG:NH2	1:A:54:THR:CG2	2.38	0.86
1:D:81:ASN:HB3	1:D:84:LEU:HB2	1.56	0.86
1:D:50:ILE:CG1	1:D:50:ILE:CG2	2.55	0.85
1:B:50:ILE:HD12	1:B:52:ARG:HG2	1.57	0.85
1:D:50:ILE:HG13	1:D:66:LEU:HD11	1.57	0.85
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.39	0.85
1:D:50:ILE:HD13	1:D:62:GLU:HB3	1.57	0.85
1:C:16:LYS:HE3	1:C:56:GLY:HA3	1.59	0.84
1:B:52:ARG:NH1	1:B:54:THR:HG21	1.90	0.84
1:C:52:ARG:HG3	2:C:171:HOH:O	1.77	0.84
1:A:1:MET:HB3	2:A:168:HOH:O	1.77	0.84
1:A:2:ASN:ND2	1:A:5:GLU:HG2	1.91	0.84
1:C:32:LEU:CB	1:C:32:LEU:CD2	2.55	0.84
1:D:2:ASN:ND2	1:D:4:PHE:HB3	1.90	0.83
1:A:111:VAL:HA	1:A:114:PHE:CE1	2.14	0.83
1:C:34:THR:CG2	1:C:34:THR:O	2.28	0.82
1:B:52:ARG:CG	1:B:54:THR:HG23	2.10	0.82
1:C:80:ARG:HG2	1:C:80:ARG:HH11	1.45	0.82
1:B:52:ARG:NH1	1:B:54:THR:CG2	2.42	0.82
1:B:50:ILE:CD1	1:B:54:THR:HG21	2.09	0.82
1:C:24:TYR:CE1	1:C:35:LYS:HG3	2.13	0.82
1:D:126:TRP:CE3	1:D:126:TRP:HA	2.14	0.81
1:B:50:ILE:CD1	1:B:52:ARG:HG2	2.10	0.81
1:C:19:LYS:HZ2	1:C:19:LYS:HB3	1.45	0.81
1:A:24:TYR:CZ	1:A:35:LYS:HG2	2.16	0.81
1:A:32:LEU:HD12	1:A:33:LEU:H	1.45	0.80
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ARG:HG3	1:C:52:ARG:HH11	1.47	0.80
1:D:6:MET:HE1	1:D:101:ASN:CB	2.11	0.80
1:D:76:ARG:HA	1:D:79:LEU:HD12	1.62	0.80
1:A:52:ARG:NH1	1:A:54:THR:HG23	1.95	0.80
1:A:52:ARG:NH2	1:A:54:THR:HG22	1.96	0.79
1:A:17:ILE:HD12	1:A:27:ILE:HD12	1.65	0.79
1:D:78:ILE:HG12	1:D:84:LEU:HD13	1.65	0.79
1:A:85:LYS:HB3	1:A:86:PRO:HD3	1.66	0.78
1:B:24:TYR:CE2	1:B:35:LYS:HE2	2.17	0.78
1:D:83:LYS:O	1:D:84:LEU:HD23	1.84	0.78
1:C:4:PHE:HE2	1:C:60:LYS:HE3	1.48	0.78
1:C:5:GLU:HG3	1:C:8:ARG:NH1	1.98	0.78
1:D:120:MET:HA	1:D:123:GLN:HB2	1.65	0.77
1:C:13:LEU:HD11	1:C:15:LEU:HD21	1.64	0.77
1:C:101:ASN:ND2	1:C:145:ARG:HH21	1.82	0.77
1:C:52:ARG:CG	1:C:54:THR:HG23	2.13	0.77
1:D:147:LYS:HE3	1:D:151:THR:HG21	1.67	0.77
1:B:6:MET:CE	1:B:101:ASN:HD22	1.98	0.76
1:B:17:ILE:HD11	1:B:25:TYR:CD1	2.21	0.76
1:C:105:GLN:HG3	1:C:145:ARG:CZ	2.15	0.76
1:D:97:ALA:HA	1:D:100:ILE:CG1	2.14	0.76
1:B:58:ILE:HB	1:B:62:GLU:HG2	1.66	0.76
1:A:120:MET:HB3	1:A:125:ARG:HB2	1.67	0.76
1:C:146:ALA:O	1:C:150:ILE:HG12	1.85	0.75
1:D:116:ASN:HA	1:D:119:ARG:HH21	1.52	0.75
1:A:52:ARG:HH12	1:A:54:THR:HA	1.52	0.75
1:B:38:SER:CB	1:B:41:ALA:HB3	2.16	0.75
1:A:83:LYS:HZ3	1:A:115:THR:HG23	1.49	0.75
1:A:144:ASN:HD21	1:B:162:LYS:HZ2	1.33	0.75
1:B:59:THR:HG22	1:B:62:GLU:N	1.99	0.75
1:D:125:ARG:CG	1:D:125:ARG:HA	2.17	0.75
1:D:52:ARG:CZ	1:D:54:THR:HG22	2.16	0.75
1:D:50:ILE:CG1	1:D:50:ILE:CA	2.65	0.75
1:B:25:TYR:O	1:B:33:LEU:HB2	1.87	0.75
1:D:127:ASP:CG	1:D:127:ASP:N	2.40	0.75
1:B:78:ILE:HG23	1:B:84:LEU:HB3	1.69	0.74
1:C:78:ILE:HD13	1:C:99:LEU:HD23	1.66	0.74
1:D:52:ARG:NE	1:D:54:THR:CG2	2.51	0.74
1:C:144:ASN:HA	1:C:147:LYS:CE	2.16	0.74
1:D:160:ALA:O	1:D:164:LEU:HB2	1.87	0.74
1:B:47:ASP:HA	1:B:50:ILE:CG2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:HG3	1:B:54:THR:CG2	2.17	0.74
1:B:59:THR:CG2	1:B:62:GLU:H	2.01	0.74
1:B:52:ARG:HG3	1:B:54:THR:HG23	1.69	0.73
1:C:157:THR:CG2	1:C:159:ASP:H	1.99	0.73
1:A:33:LEU:HG	2:A:169:HOH:O	1.88	0.73
1:C:142:THR:N	2:C:166:HOH:O	2.21	0.73
1:B:74:ALA:O	1:B:78:ILE:HG13	1.88	0.73
1:C:78:ILE:HD13	1:C:99:LEU:CD2	2.18	0.73
1:B:59:THR:HG23	1:B:61:ASP:N	2.02	0.73
1:C:120:MET:HA	1:C:125:ARG:HD3	1.70	0.73
1:C:95:ARG:HG3	1:C:153:PHE:CD1	2.23	0.73
1:C:4:PHE:CE2	1:C:60:LYS:HE3	2.23	0.73
1:C:8:ARG:O	1:C:11:GLU:O	2.07	0.73
1:D:97:ALA:HA	1:D:100:ILE:HD11	1.68	0.73
1:D:116:ASN:HA	1:D:119:ARG:HE	1.52	0.73
1:B:16:LYS:NZ	1:D:89:ASP:HB2	2.04	0.73
1:D:15:LEU:O	1:D:27:ILE:HD11	1.88	0.72
1:D:137:ARG:HG3	1:D:141:GLN:NE2	2.04	0.72
1:D:116:ASN:HA	1:D:119:ARG:NH2	2.03	0.72
1:B:17:ILE:HD12	1:B:18:TYR:N	2.03	0.72
1:C:65:LYS:N	1:C:65:LYS:HD2	2.04	0.72
1:A:144:ASN:HD21	1:B:162:LYS:HZ3	1.37	0.72
1:C:154:ARG:HH11	1:C:154:ARG:CB	2.01	0.72
1:C:159:ASP:HA	1:C:162:LYS:HG2	1.71	0.72
1:A:111:VAL:HA	1:A:114:PHE:HE1	1.54	0.72
1:D:124:LYS:CG	1:D:124:LYS:CA	2.67	0.71
1:D:125:ARG:CA	1:D:125:ARG:HG2	2.20	0.71
1:D:155:THR:O	1:D:157:THR:HG22	1.89	0.71
1:A:19:LYS:HA	1:A:24:TYR:O	1.90	0.71
1:A:116:ASN:O	1:A:120:MET:HE2	1.90	0.71
1:B:52:ARG:CD	1:B:54:THR:HG22	2.19	0.71
1:D:3:ILE:HG13	1:D:100:ILE:HD11	1.72	0.71
1:D:52:ARG:HG3	1:D:52:ARG:NH1	2.02	0.71
1:C:101:ASN:HD21	1:C:145:ARG:NH2	1.87	0.71
1:D:19:LYS:HG2	1:D:23:GLY:HA2	1.73	0.71
1:B:50:ILE:HD11	1:B:52:ARG:HH11	1.57	0.70
1:C:124:LYS:HD2	1:C:126:TRP:CZ2	2.26	0.70
1:D:48:LYS:NZ	1:D:48:LYS:HB3	2.05	0.70
1:D:116:ASN:HA	1:D:119:ARG:NE	2.05	0.70
1:D:85:LYS:N	1:D:86:PRO:HD2	2.06	0.70
1:D:97:ALA:HA	1:D:100:ILE:CD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:HG22	1:A:57:VAL:O	1.92	0.70
1:B:75:VAL:O	1:B:79:LEU:HG	1.91	0.70
1:C:3:ILE:HG23	1:C:67:PHE:CZ	2.27	0.70
1:C:114:PHE:C	1:C:118:LEU:HD12	2.11	0.70
1:A:52:ARG:HH22	1:A:54:THR:HG22	1.56	0.70
1:B:52:ARG:CG	1:B:54:THR:HG22	2.21	0.70
1:D:17:ILE:HD12	1:D:17:ILE:H	1.57	0.70
1:D:126:TRP:HA	1:D:126:TRP:HE3	1.52	0.70
1:D:147:LYS:HE3	1:D:151:THR:CG2	2.22	0.70
1:B:59:THR:H	1:B:62:GLU:HB2	1.55	0.70
1:B:52:ARG:HG2	1:B:54:THR:CG2	2.21	0.69
1:D:114:PHE:O	1:D:118:LEU:HB2	1.91	0.69
1:A:88:TYR:HA	1:A:91:LEU:HD12	1.74	0.69
1:D:52:ARG:O	1:D:52:ARG:CG	2.28	0.69
1:B:39:LEU:O	1:B:43:LYS:HB2	1.93	0.69
1:B:5:GLU:O	1:B:9:ILE:HG12	1.93	0.69
1:C:58:ILE:HD12	1:C:63:ALA:CB	2.14	0.69
1:B:69:GLN:HG3	1:B:70:ASP:N	2.08	0.69
1:D:43:LYS:HG2	1:D:55:ASN:O	1.92	0.69
1:D:79:LEU:HA	1:D:85:LYS:HG2	1.75	0.68
1:C:141:GLN:N	2:C:166:HOH:O	2.25	0.68
1:B:151:THR:HG23	1:B:155:THR:HG21	1.73	0.68
1:D:86:PRO:HB2	1:D:122:GLN:NE2	2.08	0.68
1:B:26:THR:HG22	1:B:32:LEU:HD23	1.74	0.68
1:D:97:ALA:HA	1:D:100:ILE:HG13	1.75	0.68
1:D:138:TRP:CH2	1:D:150:ILE:HD11	2.29	0.68
1:D:125:ARG:HB3	1:D:128:GLU:HG3	0.79	0.68
1:C:16:LYS:HG3	1:C:17:ILE:N	2.09	0.68
1:B:164:LEU:N	1:B:164:LEU:HD13	2.09	0.68
1:C:20:ASP:C	1:C:22:GLU:H	1.97	0.67
1:D:119:ARG:O	1:D:123:GLN:HG3	1.94	0.67
1:C:121:LEU:HD12	1:C:126:TRP:CZ3	2.30	0.67
1:B:39:LEU:O	1:B:43:LYS:HD2	1.95	0.67
1:C:97:ALA:HA	1:C:100:ILE:HG13	1.76	0.67
1:D:52:ARG:NE	1:D:54:THR:HG22	2.09	0.67
1:A:52:ARG:NH1	1:A:54:THR:HA	2.08	0.67
1:D:83:LYS:H	1:D:83:LYS:NZ	1.92	0.67
1:D:24:TYR:HB3	1:D:32:LEU:HD21	1.77	0.67
1:C:52:ARG:HG3	1:C:54:THR:HG23	1.75	0.67
1:D:50:ILE:CG1	1:D:66:LEU:HD11	2.24	0.67
1:C:34:THR:CG2	1:C:34:THR:OG1	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ILE:HG13	1:D:100:ILE:CD1	2.25	0.66
1:D:6:MET:CE	1:D:101:ASN:HD22	2.09	0.66
1:D:80:ARG:HD2	1:D:80:ARG:N	2.04	0.66
1:D:147:LYS:O	1:D:151:THR:HG23	1.96	0.66
1:A:141:GLN:HE21	1:A:141:GLN:HA	1.59	0.66
1:D:111:VAL:HA	1:D:114:PHE:HE1	1.60	0.66
1:D:150:ILE:N	1:D:150:ILE:HD13	2.10	0.66
1:D:145:ARG:O	1:D:149:VAL:HG23	1.95	0.66
1:A:2:ASN:HD21	1:A:5:GLU:HG2	1.59	0.66
1:C:59:THR:OG1	1:C:62:GLU:HB2	1.94	0.66
1:B:19:LYS:HD2	1:B:25:TYR:CE1	2.31	0.66
1:B:52:ARG:HG2	1:B:54:THR:HG23	1.76	0.66
1:C:1:MET:HG2	1:C:4:PHE:HB3	1.76	0.66
1:C:19:LYS:HA	1:C:24:TYR:O	1.96	0.66
1:D:25:TYR:CZ	1:D:39:LEU:HD12	2.30	0.66
1:D:50:ILE:CD1	1:D:62:GLU:HB3	2.26	0.66
1:C:83:LYS:CE	1:C:115:THR:HG22	2.26	0.66
1:A:92:ASP:O	1:A:96:ARG:HG2	1.96	0.65
1:C:162:LYS:O	1:C:164:LEU:N	2.29	0.65
1:C:19:LYS:HB3	1:C:19:LYS:NZ	2.11	0.65
1:C:152:THR:O	1:C:156:GLY:N	2.29	0.65
1:D:127:ASP:CG	1:D:127:ASP:CA	2.64	0.65
1:D:10:ASP:OD2	1:D:101:ASN:ND2	2.29	0.65
1:C:78:ILE:HG21	1:C:88:TYR:CD2	2.31	0.64
1:D:66:LEU:HA	1:D:69:GLN:HG3	1.78	0.64
1:A:19:LYS:HE2	1:A:25:TYR:CZ	2.32	0.64
1:B:20:ASP:N	1:B:24:TYR:O	2.30	0.64
1:A:87:VAL:O	1:A:91:LEU:HG	1.97	0.64
1:C:78:ILE:CD1	1:C:99:LEU:HD23	2.28	0.64
1:A:94:VAL:HG11	1:A:156:GLY:C	2.18	0.64
1:A:115:THR:HA	1:A:118:LEU:HB2	1.80	0.64
1:C:16:LYS:HE3	1:C:56:GLY:CA	2.27	0.64
1:C:125:ARG:HH11	1:C:125:ARG:HG2	1.61	0.64
1:D:11:GLU:OE2	1:D:145:ARG:NH1	2.30	0.64
1:B:6:MET:HE2	1:B:101:ASN:HD22	1.62	0.64
1:C:148:ARG:HG3	1:C:148:ARG:HH11	1.62	0.64
1:D:78:ILE:CG1	1:D:84:LEU:HD13	2.28	0.64
1:C:32:LEU:CB	1:C:32:LEU:HG	2.16	0.63
1:C:13:LEU:HD22	1:C:14:ARG:N	2.13	0.63
1:C:95:ARG:HG3	1:C:153:PHE:HD1	1.62	0.63
1:D:8:ARG:HD3	1:D:9:ILE:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ALA:O	1:D:133:LEU:HB2	1.98	0.63
1:A:141:GLN:HA	1:A:141:GLN:NE2	2.13	0.63
1:C:148:ARG:HG3	1:C:148:ARG:NH1	2.14	0.63
1:B:95:ARG:HG2	1:B:153:PHE:HD1	1.64	0.63
1:D:125:ARG:NH1	1:D:128:GLU:OE2	2.31	0.63
1:C:143:PRO:O	1:C:147:LYS:HG3	1.97	0.63
1:C:52:ARG:HH12	1:C:54:THR:HA	1.64	0.63
1:C:80:ARG:HG2	1:C:80:ARG:NH1	2.12	0.63
1:D:116:ASN:HA	1:D:119:ARG:CZ	2.29	0.62
1:A:98:ALA:HB3	1:A:153:PHE:CE1	2.34	0.62
1:B:47:ASP:CA	1:B:50:ILE:HG22	2.26	0.62
1:C:1:MET:O	1:C:3:ILE:N	2.32	0.62
1:C:52:ARG:NE	1:C:62:GLU:OE2	2.29	0.62
1:D:129:ALA:O	1:D:133:LEU:N	2.30	0.62
1:C:164:LEU:N	1:C:164:LEU:HD22	2.14	0.62
1:B:113:GLY:O	1:B:115:THR:HG23	1.99	0.62
1:B:151:THR:HG23	1:B:155:THR:CG2	2.28	0.62
1:C:83:LYS:NZ	1:C:115:THR:HG22	2.14	0.62
1:B:114:PHE:O	1:B:118:LEU:HD22	1.99	0.62
1:C:3:ILE:HG23	1:C:67:PHE:HZ	1.64	0.62
1:D:81:ASN:CG	1:D:84:LEU:HG	2.20	0.62
1:C:75:VAL:HG12	1:C:100:ILE:HD13	1.81	0.62
1:C:24:TYR:CZ	1:C:35:LYS:HG3	2.34	0.61
1:C:163:ASN:C	1:C:164:LEU:HD13	2.21	0.61
1:D:24:TYR:CD1	1:D:35:LYS:HA	2.35	0.61
1:A:148:ARG:HH11	1:A:164:LEU:CD1	2.09	0.61
1:C:52:ARG:HG3	1:C:52:ARG:NH1	2.12	0.61
1:C:87:VAL:HG21	1:C:118:LEU:HB3	1.80	0.61
1:D:88:TYR:CE1	1:D:96:ARG:HD3	2.36	0.61
1:A:94:VAL:HG11	1:A:156:GLY:O	2.01	0.61
1:B:59:THR:N	1:B:62:GLU:OE1	2.33	0.61
1:C:34:THR:CG2	1:C:34:THR:C	2.69	0.61
1:C:135:LYS:NZ	1:C:135:LYS:HB3	2.14	0.61
1:B:139:TYR:N	2:B:171:HOH:O	2.34	0.61
1:D:50:ILE:CG1	1:D:50:ILE:HG23	2.31	0.61
1:A:24:TYR:CE2	1:A:35:LYS:HG2	2.36	0.61
1:D:92:ASP:OD2	1:D:95:ARG:NH1	2.30	0.61
1:D:127:ASP:O	1:D:130:ALA:N	2.33	0.61
1:B:21:THR:HG22	1:B:22:GLU:N	2.16	0.61
1:C:92:ASP:OD2	1:C:94:VAL:HG23	2.01	0.61
1:D:33:LEU:O	1:D:34:THR:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HG23	1:B:4:PHE:N	2.15	0.61
1:B:55:ASN:O	1:B:57:VAL:HG12	2.01	0.61
1:D:11:GLU:HB2	1:D:29:ILE:HG23	1.82	0.61
1:D:151:THR:O	1:D:155:THR:HG23	2.01	0.61
1:B:163:ASN:HB3	2:B:168:HOH:O	2.01	0.61
1:A:96:ARG:O	1:A:100:ILE:HG13	2.00	0.61
1:B:123:GLN:OE1	1:B:125:ARG:NH1	2.34	0.60
1:D:27:ILE:HG12	1:D:28:GLY:H	1.65	0.60
1:C:163:ASN:CG	1:C:164:LEU:HD22	2.22	0.60
1:B:20:ASP:OD1	1:B:21:THR:N	2.34	0.60
1:B:57:VAL:HG11	1:D:124:LYS:HZ1	1.66	0.60
1:C:60:LYS:O	1:C:64:GLU:HB2	2.01	0.60
1:D:14:ARG:O	1:D:28:GLY:HA2	2.01	0.60
1:D:44:SER:O	1:D:48:LYS:NZ	2.34	0.60
1:D:47:ASP:O	1:D:51:GLY:HA2	2.01	0.60
1:C:121:LEU:HD12	1:C:126:TRP:HZ3	1.65	0.60
1:C:158:LEU:N	2:C:175:HOH:O	2.27	0.60
1:A:75:VAL:HG12	1:A:76:ARG:N	2.15	0.60
1:B:55:ASN:O	1:B:57:VAL:N	2.30	0.60
1:B:83:LYS:H	1:B:83:LYS:HD3	1.67	0.60
1:B:92:ASP:OD2	1:B:94:VAL:HG23	2.01	0.60
1:A:52:ARG:NH1	1:A:54:THR:CG2	2.61	0.60
1:A:83:LYS:HZ1	1:A:115:THR:HG23	1.61	0.60
1:A:138:TRP:CZ2	1:A:146:ALA:HA	2.35	0.60
1:D:52:ARG:O	1:D:54:THR:HG23	2.02	0.60
1:C:27:ILE:HD11	1:C:58:ILE:HG12	1.84	0.60
1:D:17:ILE:HD12	1:D:17:ILE:N	2.16	0.60
1:B:137:ARG:NH2	1:C:141:GLN:HA	2.17	0.59
1:D:6:MET:HE2	1:D:101:ASN:HD22	1.66	0.59
1:B:125:ARG:NH1	1:B:125:ARG:HG3	2.15	0.59
1:C:125:ARG:HG2	1:C:125:ARG:NH1	2.17	0.59
1:A:133:LEU:HD13	1:A:150:ILE:HG13	1.84	0.59
1:B:158:LEU:HD23	2:B:165:HOH:O	2.01	0.59
1:C:11:GLU:HG3	1:C:145:ARG:HH12	1.67	0.59
1:B:125:ARG:HG3	1:B:125:ARG:HH11	1.67	0.59
1:C:26:THR:HG22	1:C:27:ILE:N	2.18	0.59
1:B:158:LEU:HD23	1:B:158:LEU:H	1.68	0.59
1:C:143:PRO:HD3	2:C:166:HOH:O	2.03	0.59
1:A:32:LEU:HD12	1:A:33:LEU:N	2.16	0.58
1:D:8:ARG:HH11	1:D:9:ILE:CD1	2.16	0.58
1:A:137:ARG:H	1:A:137:ARG:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLN:OE1	1:B:94:VAL:HG21	2.01	0.58
1:C:16:LYS:HG3	1:C:17:ILE:H	1.68	0.58
1:D:16:LYS:O	1:D:27:ILE:HG13	2.03	0.58
1:D:91:LEU:HD13	1:D:95:ARG:C	2.23	0.58
1:D:116:ASN:CA	1:D:119:ARG:HH21	2.15	0.58
1:B:92:ASP:OD1	1:B:95:ARG:HB2	2.03	0.58
1:B:8:ARG:HG3	1:B:8:ARG:O	2.03	0.58
1:B:4:PHE:HA	1:B:67:PHE:CE2	2.38	0.58
1:B:14:ARG:HD2	1:B:18:TYR:CD2	2.37	0.58
1:C:114:PHE:O	1:C:118:LEU:CG	2.51	0.58
1:D:72:ASP:O	1:D:75:VAL:HG12	2.04	0.58
1:D:107:GLY:O	1:D:111:VAL:HG23	2.04	0.58
1:D:126:TRP:CE3	1:D:126:TRP:CA	2.87	0.58
1:B:129:ALA:O	1:B:133:LEU:HG	2.03	0.58
1:B:163:ASN:O	1:B:164:LEU:HD22	2.04	0.58
1:A:19:LYS:HE2	1:A:25:TYR:CE1	2.39	0.58
1:B:47:ASP:OD2	1:B:53:ASN:HA	2.04	0.57
1:C:161:TYR:HB2	1:C:162:LYS:HZ3	1.69	0.57
1:D:50:ILE:HG22	1:D:50:ILE:O	2.04	0.57
1:C:103:VAL:O	1:C:107:GLY:N	2.33	0.57
1:D:39:LEU:O	1:D:43:LYS:HG3	2.03	0.57
1:D:83:LYS:H	1:D:83:LYS:HZ2	1.51	0.57
1:A:78:ILE:HG22	1:A:79:LEU:N	2.18	0.57
1:C:55:ASN:O	1:C:55:ASN:ND2	2.31	0.57
1:D:78:ILE:HA	1:D:84:LEU:HD12	1.87	0.57
1:B:19:LYS:HA	1:B:24:TYR:O	2.04	0.57
1:C:32:LEU:CG	1:C:32:LEU:HA	2.31	0.57
1:C:157:THR:HG23	2:C:175:HOH:O	2.04	0.57
1:D:126:TRP:O	1:D:127:ASP:CG	2.43	0.57
1:B:95:ARG:HG2	1:B:153:PHE:CD1	2.39	0.57
1:A:47:ASP:O	1:A:51:GLY:N	2.37	0.57
1:C:20:ASP:O	1:C:22:GLU:N	2.37	0.57
1:D:81:ASN:HB3	1:D:84:LEU:CB	2.33	0.56
1:D:120:MET:HB2	1:D:125:ARG:CB	2.35	0.56
1:A:141:GLN:HE22	1:B:157:THR:HA	1.70	0.56
1:B:163:ASN:C	1:B:164:LEU:HD22	2.25	0.56
1:C:120:MET:HG2	1:C:125:ARG:HE	1.71	0.56
1:D:27:ILE:HG12	1:D:28:GLY:N	2.20	0.56
1:D:49:ALA:N	2:D:166:HOH:O	2.38	0.56
1:C:8:ARG:NH1	2:C:177:HOH:O	2.37	0.56
1:D:88:TYR:CD1	1:D:96:ARG:HD3	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TRP:O	1:D:127:ASP:OD2	2.23	0.56
1:C:77:GLY:HA2	1:C:80:ARG:NH1	2.21	0.56
1:A:17:ILE:HD13	1:A:56:GLY:CA	2.36	0.56
1:B:13:LEU:HD12	1:B:14:ARG:N	2.19	0.56
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.20	0.56
1:C:115:THR:O	1:C:119:ARG:HG3	2.05	0.56
1:A:149:VAL:HG12	1:A:150:ILE:N	2.20	0.56
1:C:69:GLN:O	1:C:72:ASP:N	2.38	0.56
1:A:81:ASN:OD1	1:A:84:LEU:HG	2.06	0.56
1:A:137:ARG:HD2	1:A:137:ARG:N	2.21	0.56
1:B:121:LEU:HG	1:B:126:TRP:HZ3	1.70	0.56
1:C:102:MET:O	1:C:106:MET:HG2	2.05	0.56
1:D:20:ASP:HB3	1:D:26:THR:HG21	1.88	0.56
1:A:38:SER:HB3	1:A:41:ALA:CB	2.36	0.55
1:A:125:ARG:HB3	1:A:128:GLU:CG	2.37	0.55
1:A:96:ARG:HG3	1:A:96:ARG:NH1	2.21	0.55
1:B:96:ARG:O	1:B:100:ILE:HG12	2.07	0.55
1:B:76:ARG:O	1:B:80:ARG:HB2	2.07	0.55
1:C:67:PHE:O	1:C:71:VAL:HG12	2.06	0.55
1:A:125:ARG:HB3	1:A:128:GLU:HG3	1.87	0.55
1:B:6:MET:HE2	1:B:101:ASN:ND2	2.21	0.55
1:A:137:ARG:H	1:A:137:ARG:CD	2.20	0.55
1:D:82:ALA:HB3	1:D:83:LYS:HD3	1.89	0.55
1:A:54:THR:CG2	1:A:57:VAL:O	2.55	0.54
1:D:92:ASP:O	1:D:96:ARG:HG3	2.07	0.54
1:B:4:PHE:HA	1:B:67:PHE:CZ	2.42	0.54
1:B:38:SER:HB3	1:B:41:ALA:HB3	1.87	0.54
1:B:59:THR:N	1:B:62:GLU:HB2	2.22	0.54
1:B:119:ARG:O	1:B:123:GLN:HG3	2.08	0.54
1:A:148:ARG:HG3	1:A:160:ALA:HB1	1.88	0.54
1:B:14:ARG:O	1:B:28:GLY:HA2	2.08	0.54
1:C:100:ILE:O	1:C:104:PHE:HB2	2.07	0.54
1:D:114:PHE:CD1	1:D:114:PHE:N	2.74	0.54
1:B:17:ILE:HD11	1:B:25:TYR:HD1	1.69	0.54
1:C:60:LYS:O	1:C:60:LYS:HG2	2.08	0.54
1:C:65:LYS:O	1:C:69:GLN:HG3	2.06	0.54
1:B:27:ILE:HG22	1:B:33:LEU:HD13	1.89	0.54
1:B:57:VAL:HG11	1:D:124:LYS:NZ	2.22	0.54
1:C:120:MET:HG2	1:C:125:ARG:NE	2.22	0.54
1:A:21:THR:HA	1:B:2:ASN:HA	1.90	0.54
1:A:148:ARG:NH1	1:A:164:LEU:HD13	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:O	1:B:46:LEU:HB3	2.07	0.54
1:B:50:ILE:HD12	1:B:54:THR:HG23	1.82	0.53
1:C:69:GLN:O	1:C:72:ASP:HB2	2.09	0.53
1:C:77:GLY:N	1:C:80:ARG:HH12	2.06	0.53
1:D:143:PRO:HD2	1:D:144:ASN:OD1	2.08	0.53
1:B:58:ILE:HG13	1:B:62:GLU:CB	2.32	0.53
1:C:157:THR:HG23	1:C:158:LEU:N	2.22	0.53
1:D:39:LEU:O	1:D:43:LYS:N	2.41	0.53
1:B:137:ARG:HH22	1:C:141:GLN:HA	1.72	0.53
1:D:118:LEU:O	1:D:121:LEU:HB2	2.09	0.53
1:D:85:LYS:C	1:D:85:LYS:HD2	2.29	0.53
1:D:159:ASP:OD1	1:D:159:ASP:N	2.40	0.53
1:C:151:THR:HA	1:C:154:ARG:HH11	1.66	0.53
1:D:88:TYR:O	1:D:91:LEU:HB2	2.09	0.53
1:D:133:LEU:HD22	1:D:138:TRP:HZ3	1.74	0.53
1:B:120:MET:HB3	1:B:129:ALA:HB2	1.91	0.53
1:D:94:VAL:HG21	1:D:156:GLY:O	2.08	0.53
1:C:21:THR:O	1:C:21:THR:OG1	2.27	0.53
1:D:45:GLU:HA	1:D:48:LYS:HZ2	1.74	0.53
1:A:120:MET:HA	1:A:125:ARG:HG3	1.90	0.52
1:A:144:ASN:ND2	1:B:162:LYS:NZ	2.45	0.52
1:D:86:PRO:HB2	1:D:122:GLN:HE22	1.74	0.52
1:A:51:GLY:O	1:A:52:ARG:HB3	2.09	0.52
1:D:120:MET:HB2	1:D:125:ARG:HB2	1.91	0.52
1:B:18:TYR:O	1:B:25:TYR:HA	2.10	0.52
1:D:152:THR:O	1:D:156:GLY:N	2.43	0.52
1:B:80:ARG:HH11	1:B:80:ARG:CG	2.19	0.52
1:B:151:THR:CG2	1:B:155:THR:HG21	2.39	0.52
1:C:13:LEU:HD22	1:C:13:LEU:C	2.30	0.52
1:D:114:PHE:H	1:D:114:PHE:HD1	1.58	0.52
1:B:52:ARG:NE	1:B:54:THR:CG2	2.47	0.52
1:C:1:MET:CE	1:C:4:PHE:HD2	2.23	0.52
1:D:91:LEU:HD13	1:D:95:ARG:O	2.10	0.52
1:D:124:LYS:CB	1:D:124:LYS:CD	2.83	0.52
1:D:83:LYS:HZ3	1:D:83:LYS:HB2	1.73	0.52
1:B:14:ARG:HB2	1:B:18:TYR:HE2	1.75	0.52
1:D:4:PHE:CZ	1:D:64:GLU:HG2	2.45	0.52
1:B:14:ARG:HB2	1:B:18:TYR:CE2	2.44	0.52
1:B:50:ILE:CD1	1:B:52:ARG:HH11	2.21	0.52
1:D:101:ASN:OD1	1:D:145:ARG:NH2	2.42	0.52
1:D:119:ARG:C	1:D:123:GLN:HG3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLN:HE21	1:A:141:GLN:CA	2.23	0.52
1:D:50:ILE:CG2	1:D:50:ILE:CD1	2.87	0.52
1:A:4:PHE:HA	1:A:67:PHE:CZ	2.45	0.52
1:B:38:SER:HB2	1:B:41:ALA:HB3	1.91	0.52
1:C:83:LYS:HE2	1:C:112:ALA:O	2.10	0.52
1:A:92:ASP:OD1	1:A:95:ARG:HD2	2.10	0.51
1:C:151:THR:O	1:C:155:THR:N	2.31	0.51
1:A:105:GLN:HG2	1:A:106:MET:N	2.24	0.51
1:A:114:PHE:O	1:A:118:LEU:HG	2.10	0.51
1:A:133:LEU:HD13	1:A:150:ILE:CG1	2.40	0.51
1:B:24:TYR:N	1:B:24:TYR:CD1	2.78	0.51
1:C:32:LEU:HA	1:C:32:LEU:CD1	2.41	0.51
1:C:81:ASN:OD1	1:C:84:LEU:N	2.30	0.51
1:D:6:MET:HE2	1:D:101:ASN:ND2	2.24	0.51
1:D:29:ILE:O	1:D:29:ILE:HG22	2.09	0.51
1:A:20:ASP:CG	1:A:24:TYR:HB2	2.31	0.51
1:A:139:TYR:O	1:A:143:PRO:HB3	2.10	0.51
1:A:64:GLU:HA	1:A:67:PHE:HB3	1.93	0.51
1:D:50:ILE:CG1	1:D:50:ILE:HA	2.39	0.51
1:D:64:GLU:O	1:D:68:ASN:OD1	2.29	0.51
1:A:138:TRP:CH2	1:A:146:ALA:HA	2.46	0.51
1:C:77:GLY:HA2	1:C:80:ARG:HH12	1.75	0.51
1:D:7:LEU:O	1:D:11:GLU:O	2.29	0.51
1:C:95:ARG:CD	1:C:153:PHE:HA	2.41	0.51
1:B:137:ARG:NH2	1:C:140:ASN:O	2.43	0.51
1:D:84:LEU:O	1:D:87:VAL:HG23	2.11	0.51
1:B:29:ILE:HG22	1:B:29:ILE:O	2.11	0.51
1:B:99:LEU:O	1:B:99:LEU:HD12	2.11	0.51
1:D:50:ILE:HD11	1:D:66:LEU:CD1	2.41	0.51
1:D:87:VAL:O	1:D:90:SER:HB3	2.10	0.51
1:B:106:MET:HE2	1:B:138:TRP:CD1	2.46	0.50
1:A:86:PRO:O	1:A:90:SER:OG	2.29	0.50
1:C:35:LYS:NZ	2:C:174:HOH:O	2.41	0.50
1:A:52:ARG:O	1:A:54:THR:N	2.44	0.50
1:A:130:ALA:O	1:A:133:LEU:HB2	2.11	0.50
1:A:160:ALA:O	1:A:163:ASN:ND2	2.44	0.50
1:D:84:LEU:H	1:D:86:PRO:HD2	1.76	0.50
1:B:108:GLU:HG3	1:B:109:THR:N	2.27	0.50
1:C:14:ARG:CG	1:C:14:ARG:HH11	2.24	0.50
1:D:96:ARG:O	1:D:99:LEU:HB3	2.12	0.50
1:D:147:LYS:O	1:D:147:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:HD12	1:B:18:TYR:H	1.76	0.50
1:C:19:LYS:NZ	1:C:25:TYR:CE1	2.79	0.50
1:B:139:TYR:HB3	2:B:171:HOH:O	2.12	0.50
1:C:20:ASP:C	1:C:22:GLU:N	2.65	0.50
1:D:91:LEU:HB3	1:D:96:ARG:HG2	1.94	0.50
1:D:127:ASP:O	1:D:128:GLU:C	2.50	0.50
1:B:140:ASN:N	2:B:171:HOH:O	2.23	0.49
1:B:146:ALA:O	1:B:150:ILE:HD12	2.12	0.49
1:C:163:ASN:N	2:C:169:HOH:O	2.29	0.49
1:D:47:ASP:OD1	1:D:54:THR:O	2.31	0.49
1:D:87:VAL:HA	1:D:122:GLN:HG3	1.93	0.49
1:A:144:ASN:ND2	1:B:162:LYS:HZ2	2.06	0.49
1:B:85:LYS:HB3	1:B:86:PRO:HD3	1.95	0.49
1:B:87:VAL:O	1:B:91:LEU:HG	2.12	0.49
1:C:1:MET:SD	1:C:5:GLU:N	2.85	0.49
1:C:13:LEU:HD11	1:C:15:LEU:CD2	2.39	0.49
1:B:137:ARG:CD	2:B:172:HOH:O	2.60	0.49
1:C:81:ASN:OD1	1:C:83:LYS:N	2.45	0.49
1:D:45:GLU:HA	1:D:48:LYS:NZ	2.28	0.49
1:D:87:VAL:N	1:D:122:GLN:HE21	2.10	0.49
1:B:6:MET:HG2	1:B:7:LEU:N	2.26	0.49
1:B:47:ASP:OD1	1:B:54:THR:O	2.30	0.49
1:D:82:ALA:CB	1:D:83:LYS:HD3	2.43	0.49
1:A:114:PHE:H	1:A:114:PHE:HD1	1.56	0.49
1:C:77:GLY:CA	1:C:80:ARG:HH12	2.26	0.49
1:D:7:LEU:O	1:D:11:GLU:N	2.46	0.49
1:D:119:ARG:HB3	1:D:123:GLN:HE21	1.78	0.49
1:C:4:PHE:CE1	1:C:29:ILE:HD11	2.48	0.49
1:C:54:THR:HB	1:C:57:VAL:O	2.12	0.49
1:C:87:VAL:O	1:C:91:LEU:HG	2.12	0.49
1:D:68:ASN:O	1:D:72:ASP:OD2	2.30	0.49
1:D:81:ASN:OD1	1:D:83:LYS:NZ	2.45	0.49
1:C:50:ILE:CG2	1:C:52:ARG:HG2	2.43	0.49
1:C:114:PHE:O	1:C:118:LEU:HG	2.13	0.49
1:C:151:THR:O	1:C:155:THR:HG23	2.13	0.49
1:C:161:TYR:CD1	1:C:161:TYR:N	2.79	0.49
1:A:52:ARG:O	1:A:52:ARG:HG3	2.13	0.48
1:C:120:MET:CG	1:C:125:ARG:HE	2.26	0.48
1:D:94:VAL:HG23	1:D:94:VAL:O	2.13	0.48
1:C:51:GLY:O	1:C:52:ARG:HB3	2.14	0.48
1:D:116:ASN:CB	1:D:119:ARG:HH21	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD12	1:B:126:TRP:CZ3	2.49	0.48
1:D:83:LYS:HD3	1:D:83:LYS:N	2.29	0.48
1:A:46:LEU:HD22	1:A:50:ILE:HG12	1.94	0.48
1:A:141:GLN:HE22	1:B:157:THR:CA	2.26	0.48
1:B:106:MET:HE2	1:B:138:TRP:NE1	2.29	0.48
1:C:81:ASN:CG	1:C:84:LEU:HD22	2.33	0.48
1:D:7:LEU:HA	1:D:10:ASP:HB2	1.95	0.48
1:D:65:LYS:O	1:D:69:GLN:HG2	2.13	0.48
1:D:105:GLN:OE1	1:D:138:TRP:NE1	2.46	0.48
1:A:38:SER:HB3	1:A:41:ALA:HB3	1.96	0.48
1:B:121:LEU:HD12	1:B:126:TRP:CE3	2.49	0.48
1:D:6:MET:CE	1:D:101:ASN:ND2	2.76	0.48
1:D:17:ILE:H	1:D:17:ILE:CD1	2.13	0.48
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.78	0.48
1:B:155:THR:C	1:B:157:THR:H	2.16	0.48
1:D:32:LEU:C	1:D:33:LEU:HD12	2.33	0.48
1:D:95:ARG:CZ	1:D:126:TRP:CZ2	2.97	0.48
1:D:95:ARG:NH2	1:D:156:GLY:HA3	2.29	0.48
1:D:144:ASN:OD1	1:D:144:ASN:N	2.42	0.48
1:B:52:ARG:CD	1:B:54:THR:CG2	2.88	0.48
1:D:50:ILE:CG2	1:D:50:ILE:HD13	2.44	0.48
1:B:17:ILE:CD1	1:B:25:TYR:CD1	2.93	0.47
1:D:77:GLY:O	1:D:81:ASN:N	2.46	0.47
1:D:78:ILE:CG2	1:D:84:LEU:HB3	2.29	0.47
1:D:111:VAL:O	1:D:114:PHE:HD1	1.97	0.47
1:B:16:LYS:HZ1	1:D:89:ASP:HB2	1.79	0.47
1:B:27:ILE:CG2	1:B:33:LEU:HD13	2.44	0.47
1:B:52:ARG:HG3	1:B:54:THR:HG22	1.91	0.47
1:B:13:LEU:HA	1:B:28:GLY:O	2.15	0.47
1:B:59:THR:HG23	1:B:60:LYS:N	2.30	0.47
1:B:126:TRP:CB	1:B:154:ARG:HA	2.31	0.47
1:D:85:LYS:N	1:D:86:PRO:CD	2.77	0.47
1:A:17:ILE:HD13	1:A:56:GLY:HA2	1.96	0.47
1:A:116:ASN:ND2	1:A:117:SER:H	2.11	0.47
1:B:95:ARG:NH2	1:B:156:GLY:CA	2.78	0.47
1:D:125:ARG:HG2	1:D:125:ARG:N	2.29	0.47
1:B:21:THR:C	1:B:23:GLY:H	2.17	0.47
1:B:121:LEU:C	1:B:123:GLN:H	2.16	0.47
1:A:129:ALA:O	1:A:133:LEU:HG	2.14	0.47
1:A:143:PRO:HD2	1:A:144:ASN:H	1.79	0.47
1:B:3:ILE:CG2	1:B:4:PHE:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PHE:CE2	1:B:64:GLU:HG3	2.49	0.47
1:B:51:GLY:O	1:B:52:ARG:HB3	2.14	0.47
1:B:79:LEU:HA	1:B:85:LYS:CG	2.35	0.47
1:C:158:LEU:O	1:C:162:LYS:HE2	2.14	0.47
1:C:163:ASN:OD1	1:C:164:LEU:HD22	2.13	0.47
1:A:54:THR:O	1:A:55:ASN:HB3	2.14	0.47
1:A:83:LYS:HZ3	1:A:115:THR:CG2	2.25	0.47
1:B:50:ILE:HD13	1:B:50:ILE:O	2.14	0.47
1:C:26:THR:CG2	1:C:27:ILE:N	2.77	0.47
1:D:66:LEU:O	1:D:70:ASP:HB2	2.14	0.47
1:D:116:ASN:OD1	1:D:117:SER:N	2.43	0.47
1:D:128:GLU:H	1:D:128:GLU:HG2	1.37	0.47
1:B:80:ARG:NH1	1:B:80:ARG:CG	2.78	0.47
1:B:125:ARG:HH11	1:B:125:ARG:CG	2.28	0.47
1:D:43:LYS:HE3	1:D:55:ASN:O	2.15	0.47
1:C:83:LYS:HE3	1:C:115:THR:CB	2.46	0.46
1:C:159:ASP:N	2:C:175:HOH:O	2.49	0.46
1:A:21:THR:HG22	1:B:1:MET:O	2.15	0.46
1:D:133:LEU:O	1:D:136:SER:OG	2.27	0.46
1:D:95:ARG:HD2	1:D:126:TRP:CH2	2.50	0.46
1:D:124:LYS:HG2	1:D:124:LYS:N	2.30	0.46
1:A:141:GLN:O	1:A:143:PRO:HD3	2.16	0.46
1:D:154:ARG:HG3	1:D:155:THR:N	2.31	0.46
1:A:26:THR:HB	1:A:31:HIS:O	2.14	0.46
1:B:163:ASN:ND2	1:B:164:LEU:CD2	2.78	0.46
1:C:71:VAL:O	1:C:75:VAL:HG22	2.16	0.46
1:D:88:TYR:CE1	1:D:96:ARG:CD	2.98	0.46
1:B:8:ARG:HA	1:B:29:ILE:HD13	1.98	0.46
1:B:17:ILE:CG2	1:B:56:GLY:HA2	2.46	0.46
1:C:50:ILE:HG13	1:C:62:GLU:CG	2.25	0.46
1:A:17:ILE:CD1	1:A:27:ILE:HD12	2.41	0.46
1:B:6:MET:CE	1:B:101:ASN:ND2	2.73	0.46
1:D:5:GLU:HA	1:D:8:ARG:HB3	1.96	0.46
1:D:67:PHE:HA	1:D:70:ASP:HB2	1.97	0.46
1:D:46:LEU:O	1:D:50:ILE:N	2.44	0.46
1:A:14:ARG:O	1:A:28:GLY:N	2.45	0.46
1:B:58:ILE:HB	1:B:62:GLU:CG	2.42	0.46
1:D:95:ARG:HD2	1:D:126:TRP:HH2	1.80	0.46
1:B:163:ASN:CG	1:B:164:LEU:HD22	2.36	0.46
1:C:5:GLU:HG3	1:C:8:ARG:HH12	1.76	0.46
1:D:40:ASN:O	1:D:44:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ARG:CD	1:D:126:TRP:CH2	2.99	0.46
1:C:3:ILE:HG23	1:C:67:PHE:CE1	2.50	0.45
1:A:143:PRO:CD	1:A:144:ASN:H	2.30	0.45
1:B:55:ASN:C	1:B:57:VAL:H	2.14	0.45
1:B:85:LYS:CB	1:B:86:PRO:HD3	2.46	0.45
1:B:151:THR:O	1:B:155:THR:OG1	2.34	0.45
1:C:49:ALA:HA	2:C:167:HOH:O	2.16	0.45
1:D:102:MET:HG2	1:D:106:MET:HE2	1.97	0.45
1:B:17:ILE:CD1	1:B:25:TYR:HD1	2.28	0.45
1:B:119:ARG:HG3	1:B:120:MET:N	2.30	0.45
1:C:101:ASN:C	1:C:101:ASN:HD22	2.18	0.45
1:D:60:LYS:HE2	1:D:60:LYS:HB3	1.42	0.45
1:A:141:GLN:C	1:A:143:PRO:HD3	2.37	0.45
1:B:152:THR:HA	1:B:155:THR:OG1	2.17	0.45
1:C:27:ILE:O	1:C:31:HIS:HB3	2.16	0.45
1:C:95:ARG:CG	1:C:153:PHE:HD1	2.29	0.45
1:C:99:LEU:O	1:C:103:VAL:HG23	2.16	0.45
1:C:131:VAL:HG22	1:C:132:ASN:N	2.31	0.45
1:C:147:LYS:HG3	1:C:147:LYS:H	1.58	0.45
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.77	0.45
1:B:121:LEU:CD1	1:B:126:TRP:CE3	2.99	0.45
1:B:163:ASN:ND2	1:B:164:LEU:HD22	2.31	0.45
1:B:163:ASN:HD22	1:B:164:LEU:HD13	1.82	0.45
1:C:26:THR:HG23	1:C:31:HIS:O	2.17	0.45
1:D:4:PHE:HD1	1:D:67:PHE:CE1	2.34	0.45
1:D:9:ILE:HG22	1:D:148:ARG:NH2	2.32	0.45
1:B:157:THR:OG1	1:B:159:ASP:OD1	2.34	0.45
1:C:52:ARG:HG2	1:C:54:THR:HG23	1.98	0.45
1:C:68:ASN:O	1:C:71:VAL:HG13	2.17	0.45
1:A:31:HIS:HD2	2:A:169:HOH:O	2.00	0.45
1:D:135:LYS:HD2	1:D:135:LYS:HA	1.54	0.45
1:D:44:SER:O	1:D:48:LYS:HB3	2.17	0.44
1:C:14:ARG:CG	1:C:14:ARG:NH1	2.79	0.44
1:C:95:ARG:HD2	1:C:153:PHE:O	2.17	0.44
1:B:123:GLN:HB2	1:B:125:ARG:NH1	2.32	0.44
1:C:61:ASP:N	1:C:61:ASP:OD1	2.49	0.44
1:C:121:LEU:HD12	1:C:126:TRP:CE3	2.52	0.44
1:D:41:ALA:O	1:D:45:GLU:HB2	2.17	0.44
1:D:124:LYS:CG	1:D:124:LYS:N	2.80	0.44
1:A:78:ILE:HD11	1:A:103:VAL:HG21	1.99	0.44
1:D:31:HIS:HD2	1:D:33:LEU:HD11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:HD1	1:B:153:PHE:HA	1.61	0.44
1:D:91:LEU:HD23	1:D:91:LEU:HA	1.80	0.44
1:D:101:ASN:O	1:D:104:PHE:HB2	2.17	0.44
1:A:13:LEU:HD13	1:A:29:ILE:HG12	1.99	0.44
1:B:158:LEU:HD23	1:B:158:LEU:N	2.31	0.44
1:A:27:ILE:HG12	1:A:58:ILE:HD13	2.00	0.44
1:A:45:GLU:HA	1:A:48:LYS:HG3	2.00	0.44
1:A:109:THR:O	1:A:112:ALA:N	2.51	0.44
1:B:27:ILE:HG13	1:B:28:GLY:N	2.33	0.44
1:D:77:GLY:O	1:D:81:ASN:HB2	2.18	0.44
1:A:2:ASN:ND2	1:A:5:GLU:CG	2.75	0.44
1:B:57:VAL:CG1	1:D:124:LYS:NZ	2.79	0.44
1:B:87:VAL:HG21	1:B:118:LEU:HG	1.99	0.44
1:B:131:VAL:HG13	1:B:132:ASN:N	2.32	0.44
1:C:59:THR:H	1:C:62:GLU:HB2	1.82	0.44
1:C:72:ASP:HB3	1:C:76:ARG:NH1	2.32	0.44
1:A:88:TYR:HA	1:A:91:LEU:CD1	2.45	0.43
1:C:2:ASN:HA	1:C:5:GLU:HB2	2.00	0.43
1:B:50:ILE:HD13	1:B:52:ARG:HG2	1.95	0.43
1:B:59:THR:O	1:B:62:GLU:HB2	2.18	0.43
1:D:4:PHE:CE1	1:D:64:GLU:HG2	2.54	0.43
1:D:97:ALA:CA	1:D:100:ILE:HG13	2.45	0.43
1:A:20:ASP:OD2	1:A:24:TYR:HB2	2.18	0.43
1:C:85:LYS:CB	1:C:86:PRO:CD	2.97	0.43
1:D:60:LYS:O	1:D:64:GLU:HB2	2.17	0.43
1:B:50:ILE:HD11	1:B:52:ARG:NH1	2.29	0.43
1:C:148:ARG:HH11	1:C:148:ARG:CG	2.29	0.43
1:D:19:LYS:HG2	1:D:23:GLY:CA	2.46	0.43
1:A:109:THR:O	1:A:112:ALA:HB3	2.18	0.43
1:B:31:HIS:HD1	1:B:70:ASP:CG	2.20	0.43
1:C:139:TYR:HD1	1:C:146:ALA:HB1	1.83	0.43
1:D:6:MET:CE	1:D:101:ASN:HB2	2.34	0.43
1:A:22:GLU:HB3	1:B:93:ALA:HB1	2.01	0.43
1:A:133:LEU:CD1	1:A:150:ILE:HG12	2.49	0.43
1:C:115:THR:H	1:C:115:THR:HG23	1.49	0.43
1:D:84:LEU:C	1:D:86:PRO:HD2	2.38	0.43
1:B:52:ARG:HH21	1:D:124:LYS:HG3	1.83	0.43
1:A:116:ASN:ND2	1:A:117:SER:OG	2.52	0.43
1:C:114:PHE:C	1:C:118:LEU:CD1	2.78	0.43
1:B:163:ASN:ND2	1:B:164:LEU:CD1	2.82	0.43
1:A:50:ILE:HG21	1:A:62:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:ND2	1:A:108:GLU:OE2	2.37	0.42
1:A:120:MET:CE	1:A:132:ASN:ND2	2.83	0.42
1:D:31:HIS:CD2	1:D:33:LEU:CD1	3.01	0.42
1:D:62:GLU:O	1:D:65:LYS:HB3	2.19	0.42
1:B:73:ALA:O	1:B:77:GLY:N	2.43	0.42
1:A:137:ARG:HG2	1:A:138:TRP:N	2.34	0.42
1:B:123:GLN:CB	1:B:125:ARG:NH1	2.82	0.42
1:B:140:ASN:O	1:B:143:PRO:HD3	2.20	0.42
1:D:84:LEU:N	1:D:86:PRO:HD2	2.34	0.42
1:D:102:MET:HG2	1:D:106:MET:CE	2.50	0.42
1:B:66:LEU:HA	1:B:69:GLN:HG2	2.01	0.42
1:C:6:MET:HG3	1:C:161:TYR:CE2	2.55	0.42
1:C:52:ARG:NH1	1:C:54:THR:HA	2.32	0.42
1:C:26:THR:CG2	1:C:27:ILE:H	2.33	0.42
1:B:24:TYR:CD2	1:B:35:LYS:HE2	2.55	0.42
1:C:7:LEU:HD13	1:C:7:LEU:HA	1.88	0.42
1:D:26:THR:HA	1:D:33:LEU:HD13	2.00	0.42
1:A:120:MET:HE1	1:A:132:ASN:ND2	2.34	0.42
1:C:17:ILE:HG22	1:C:18:TYR:N	2.35	0.42
1:D:121:LEU:HD23	1:D:121:LEU:HA	1.82	0.42
1:D:162:LYS:HD3	1:D:162:LYS:HA	1.63	0.42
1:A:38:SER:CB	1:A:41:ALA:CB	2.97	0.42
1:C:14:ARG:HH11	1:C:14:ARG:HG3	1.85	0.42
1:C:26:THR:HG22	1:C:27:ILE:H	1.84	0.42
1:D:50:ILE:CD1	1:D:62:GLU:CB	2.96	0.42
1:D:146:ALA:O	1:D:150:ILE:HG12	2.19	0.42
1:A:17:ILE:HD12	1:A:17:ILE:N	2.35	0.41
1:D:31:HIS:CD2	1:D:33:LEU:HD11	2.55	0.41
1:B:118:LEU:O	1:B:121:LEU:HB2	2.20	0.41
1:C:38:SER:HB3	1:C:41:ALA:HB3	2.01	0.41
1:D:138:TRP:CZ3	1:D:150:ILE:HD11	2.53	0.41
1:D:50:ILE:HA	1:D:50:ILE:HG12	2.00	0.41
1:A:141:GLN:NE2	1:B:157:THR:HB	2.35	0.41
1:A:31:HIS:CD2	2:A:169:HOH:O	2.73	0.41
1:A:38:SER:HB3	1:A:41:ALA:H	1.85	0.41
1:B:59:THR:H	1:B:62:GLU:CB	2.27	0.41
1:B:159:ASP:HA	1:B:162:LYS:HB2	2.03	0.41
1:C:35:LYS:HE2	1:C:35:LYS:HB2	1.69	0.41
1:C:139:TYR:O	1:C:139:TYR:CD2	2.73	0.41
1:A:41:ALA:O	1:A:45:GLU:HG2	2.21	0.41
1:A:116:ASN:C	1:A:120:MET:HE2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:ND2	1:B:162:LYS:HZ3	2.11	0.41
1:C:102:MET:HE2	1:C:111:VAL:HG13	2.02	0.41
1:D:9:ILE:HG22	1:D:148:ARG:HH21	1.86	0.41
1:D:20:ASP:OD1	1:D:24:TYR:N	2.51	0.41
1:D:131:VAL:O	1:D:134:ALA:HB3	2.21	0.41
1:A:4:PHE:HA	1:A:67:PHE:CE2	2.56	0.41
1:A:105:GLN:CD	1:A:138:TRP:HE1	2.24	0.41
1:A:114:PHE:CD1	1:A:114:PHE:N	2.79	0.41
1:C:1:MET:SD	1:C:5:GLU:OE1	2.78	0.41
1:C:34:THR:HG23	1:C:34:THR:C	2.27	0.41
1:D:50:ILE:CG2	1:D:50:ILE:O	2.67	0.41
1:A:81:ASN:CG	1:A:84:LEU:HG	2.41	0.41
1:A:102:MET:HA	1:A:106:MET:HE3	2.02	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.80	0.41
1:B:163:ASN:ND2	1:B:164:LEU:HD13	2.36	0.41
1:C:66:LEU:O	1:C:69:GLN:HB2	2.21	0.41
1:C:83:LYS:CE	1:C:115:THR:CG2	2.97	0.41
1:A:27:ILE:CD1	1:A:58:ILE:HG23	2.51	0.40
1:C:50:ILE:HG21	1:C:52:ARG:HG2	2.03	0.40
1:B:19:LYS:HB3	1:B:19:LYS:HE2	1.23	0.40
1:C:52:ARG:CG	2:C:171:HOH:O	2.53	0.40
1:C:83:LYS:NZ	1:C:115:THR:CG2	2.83	0.40
1:B:24:TYR:N	1:B:24:TYR:HD1	2.18	0.40
1:D:87:VAL:O	1:D:90:SER:N	2.54	0.40
1:D:106:MET:O	1:D:107:GLY:O	2.39	0.40
1:A:38:SER:CB	1:A:41:ALA:HB3	2.52	0.40
1:B:32:LEU:HD23	1:B:32:LEU:HA	1.92	0.40
1:B:114:PHE:H	1:B:114:PHE:HD1	1.67	0.40
1:D:49:ALA:HB2	2:D:166:HOH:O	2.22	0.40
1:D:95:ARG:CZ	1:D:156:GLY:HA3	2.52	0.40
1:A:114:PHE:O	1:A:118:LEU:N	2.50	0.40
1:C:154:ARG:NH1	1:C:154:ARG:CB	2.78	0.40
1:C:158:LEU:HD23	1:C:158:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	143 (88%)	16 (10%)	3 (2%)	8	15
1	B	162/164 (99%)	132 (82%)	23 (14%)	7 (4%)	2	3
1	C	162/164 (99%)	136 (84%)	21 (13%)	5 (3%)	4	6
1	D	162/164 (99%)	127 (78%)	28 (17%)	7 (4%)	2	3
All	All	648/656 (99%)	538 (83%)	88 (14%)	22 (3%)	3	5

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	B	37	PRO
1	B	136	SER
1	C	21	THR
1	C	163	ASN
1	C	2	ASN
1	D	107	GLY
1	A	126	TRP
1	B	163	ASN
1	D	51	GLY
1	D	56	GLY
1	D	144	ASN
1	A	114	PHE
1	B	22	GLU
1	B	36	SER
1	D	20	ASP
1	D	148	ARG
1	B	56	GLY
1	C	69	GLN
1	C	70	ASP
1	D	160	ALA
1	B	78	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	137/137 (100%)	93 (68%)	44 (32%)	0	0
1	B	137/137 (100%)	79 (58%)	58 (42%)	0	0
1	C	137/137 (100%)	87 (64%)	50 (36%)	0	0
1	D	137/137 (100%)	75 (55%)	62 (45%)	0	0
All	All	548/548 (100%)	334 (61%)	214 (39%)	0	0

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	LEU
1	A	8	ARG
1	A	21	THR
1	A	22	GLU
1	A	26	THR
1	A	29	ILE
1	A	34	THR
1	A	38	SER
1	A	39	LEU
1	A	43	LYS
1	A	44	SER
1	A	46	LEU
1	A	48	LYS
1	A	53	ASN
1	A	54	THR
1	A	57	VAL
1	A	58	ILE
1	A	60	LYS
1	A	69	GLN
1	A	75	VAL
1	A	78	ILE
1	A	80	ARG
1	A	83	LYS

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Mol	Chain	Res	Type
1	A	90	SER
1	A	91	LEU
1	A	99	LEU
1	A	105	GLN
1	A	114	PHE
1	A	115	THR
1	A	116	ASN
1	A	117	SER
1	A	119	ARG
1	A	124	LYS
1	A	125	ARG
1	A	128	GLU
1	A	135	LYS
1	A	137	ARG
1	A	141	GLN
1	A	144	ASN
1	A	145	ARG
1	A	147	LYS
1	A	152	THR
1	A	164	LEU
1	B	3	ILE
1	B	5	GLU
1	B	6	MET
1	B	8	ARG
1	B	14	ARG
1	B	16	LYS
1	B	17	ILE
1	B	19	LYS
1	B	20	ASP
1	B	21	THR
1	B	22	GLU
1	B	27	ILE
1	B	29	ILE
1	B	32	LEU
1	B	33	LEU
1	B	36	SER
1	B	38	SER
1	B	40	ASN
1	B	44	SER
1	B	47	ASP
1	B	50	ILE
1	B	52	ARG

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Mol	Chain	Res	Type
1	B	58	ILE
1	B	59	THR
1	B	61	ASP
1	B	62	GLU
1	B	64	GLU
1	B	69	GLN
1	B	76	ARG
1	B	79	LEU
1	B	80	ARG
1	B	83	LYS
1	B	84	LEU
1	B	85	LYS
1	B	90	SER
1	B	94	VAL
1	B	106	MET
1	B	109	THR
1	B	116	ASN
1	B	118	LEU
1	B	119	ARG
1	B	121	LEU
1	B	122	GLN
1	B	125	ARG
1	B	127	ASP
1	B	135	LYS
1	B	136	SER
1	B	137	ARG
1	B	140	ASN
1	B	142	THR
1	B	145	ARG
1	B	153	PHE
1	B	157	THR
1	B	158	LEU
1	B	159	ASP
1	B	162	LYS
1	B	163	ASN
1	B	164	LEU
1	C	1	MET
1	C	2	ASN
1	C	3	ILE
1	C	7	LEU
1	C	8	ARG
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	14	ARG
1	C	15	LEU
1	C	19	LYS
1	C	21	THR
1	C	34	THR
1	C	35	LYS
1	C	39	LEU
1	C	45	GLU
1	C	50	ILE
1	C	55	ASN
1	C	57	VAL
1	C	61	ASP
1	C	62	GLU
1	C	65	LYS
1	C	71	VAL
1	C	83	LYS
1	C	84	LEU
1	C	85	LYS
1	C	94	VAL
1	C	96	ARG
1	C	99	LEU
1	C	100	ILE
1	C	101	ASN
1	C	105	GLN
1	C	108	GLU
1	C	109	THR
1	C	114	PHE
1	C	117	SER
1	C	118	LEU
1	C	121	LEU
1	C	128	GLU
1	C	135	LYS
1	C	137	ARG
1	C	140	ASN
1	C	141	GLN
1	C	144	ASN
1	C	145	ARG
1	C	147	LYS
1	C	151	THR
1	C	154	ARG
1	C	157	THR
1	C	161	TYR

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Mol	Chain	Res	Type
1	C	162	LYS
1	C	164	LEU
1	D	1	MET
1	D	2	ASN
1	D	3	ILE
1	D	8	ARG
1	D	9	ILE
1	D	15	LEU
1	D	17	ILE
1	D	19	LYS
1	D	20	ASP
1	D	26	THR
1	D	32	LEU
1	D	34	THR
1	D	35	LYS
1	D	36	SER
1	D	39	LEU
1	D	44	SER
1	D	45	GLU
1	D	48	LYS
1	D	50	ILE
1	D	52	ARG
1	D	57	VAL
1	D	59	THR
1	D	61	ASP
1	D	62	GLU
1	D	64	GLU
1	D	65	LYS
1	D	69	GLN
1	D	70	ASP
1	D	75	VAL
1	D	79	LEU
1	D	80	ARG
1	D	83	LYS
1	D	85	LYS
1	D	87	VAL
1	D	89	ASP
1	D	99	LEU
1	D	100	ILE
1	D	106	MET
1	D	108	GLU
1	D	109	THR

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Mol	Chain	Res	Type
1	D	114	PHE
1	D	115	THR
1	D	117	SER
1	D	118	LEU
1	D	120	MET
1	D	126	TRP
1	D	127	ASP
1	D	128	GLU
1	D	131	VAL
1	D	132	ASN
1	D	135	LYS
1	D	136	SER
1	D	137	ARG
1	D	142	THR
1	D	144	ASN
1	D	145	ARG
1	D	147	LYS
1	D	148	ARG
1	D	150	ILE
1	D	154	ARG
1	D	159	ASP
1	D	162	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	68	ASN
1	A	116	ASN
1	A	122	GLN
1	A	132	ASN
1	A	141	GLN
1	A	144	ASN
1	B	53	ASN
1	B	69	GLN
1	B	101	ASN
1	B	132	ASN
1	B	163	ASN
1	C	2	ASN
1	C	69	GLN
1	C	101	ASN
1	C	122	GLN

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Mol	Chain	Res	Type
1	D	31	HIS
1	D	68	ASN
1	D	69	GLN
1	D	122	GLN
1	D	123	GLN
1	D	140	ASN
1	D	141	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	126:TRP	C	127:ASP	N	1.18
1	D	50:ILE	C	51:GLY	N	1.03

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/164 (100%)	-0.72	1 (0%) 89 88	8, 28, 57, 98	0
1	B	164/164 (100%)	-0.55	0 100 100	13, 36, 66, 102	0
1	C	164/164 (100%)	-0.60	0 100 100	13, 31, 62, 109	0
1	D	164/164 (100%)	-0.28	1 (0%) 89 88	19, 49, 79, 94	0
All	All	656/656 (100%)	-0.54	2 (0%) 94 93	8, 36, 71, 109	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	LEU	5.5
1	D	164	LEU	2.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.