



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:41 pm BST

PDB ID : 1Q1B
Title : Crystal structure of E. coli MalK in the nucleotide-free form
Authors : Chen, J.; Lu, G.; Lin, J.; Davidson, A.L.; Quiocho, F.A.
Deposited on : 2003-07-18
Resolution : 2.80 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	:	2.11
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)	:	2.11

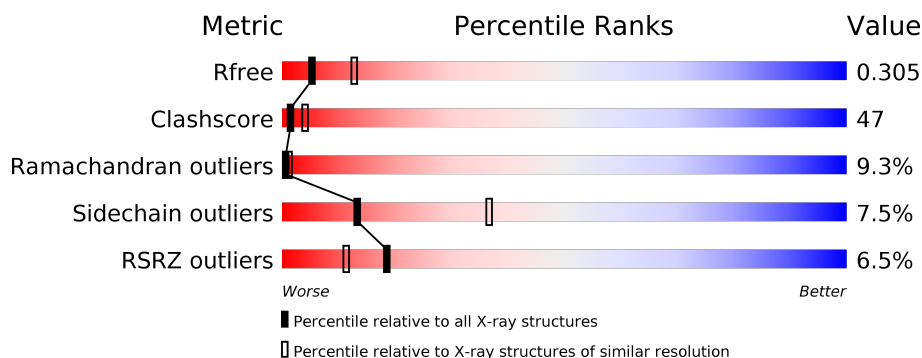
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	381	<div> <div>41%</div> <div>46%</div> <div>9%</div> <div>• •</div> </div>
1	B	381	<div> <div>18%</div> <div>33%</div> <div>47%</div> <div>15%</div> <div>• •</div> </div>
1	C	381	<div> <div>42%</div> <div>43%</div> <div>11%</div> <div>•</div> </div>
1	D	381	<div> <div>7%</div> <div>35%</div> <div>50%</div> <div>9%</div> <div>• •</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11412 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 Maltose/maltodextrin transport ATP-binding protein malK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	B	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	C	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			
1	D	367	Total	C	N	O	S	0	0	0
			2853	1805	511	524	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	GLU	-	EXPRESSION TAG	UNP P68187
A	373	SER	-	EXPRESSION TAG	UNP P68187
A	374	ALA	-	EXPRESSION TAG	UNP P68187
A	375	SER	-	EXPRESSION TAG	UNP P68187
A	376	HIS	-	EXPRESSION TAG	UNP P68187
A	377	HIS	-	EXPRESSION TAG	UNP P68187
A	378	HIS	-	EXPRESSION TAG	UNP P68187
A	379	HIS	-	EXPRESSION TAG	UNP P68187
A	380	HIS	-	EXPRESSION TAG	UNP P68187
A	381	HIS	-	EXPRESSION TAG	UNP P68187
B	372	GLU	-	EXPRESSION TAG	UNP P68187
B	373	SER	-	EXPRESSION TAG	UNP P68187
B	374	ALA	-	EXPRESSION TAG	UNP P68187
B	375	SER	-	EXPRESSION TAG	UNP P68187
B	376	HIS	-	EXPRESSION TAG	UNP P68187
B	377	HIS	-	EXPRESSION TAG	UNP P68187
B	378	HIS	-	EXPRESSION TAG	UNP P68187
B	379	HIS	-	EXPRESSION TAG	UNP P68187
B	380	HIS	-	EXPRESSION TAG	UNP P68187
B	381	HIS	-	EXPRESSION TAG	UNP P68187
C	372	GLU	-	EXPRESSION TAG	UNP P68187

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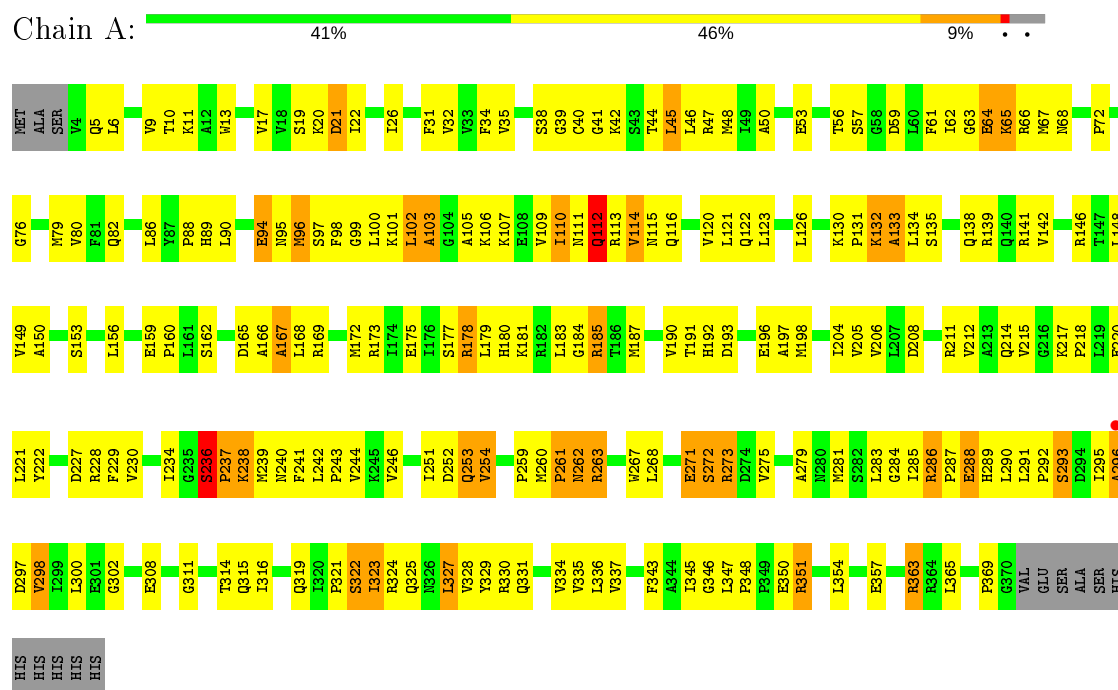
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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	SER	-	EXPRESSION TAG	UNP P68187
C	374	ALA	-	EXPRESSION TAG	UNP P68187
C	375	SER	-	EXPRESSION TAG	UNP P68187
C	376	HIS	-	EXPRESSION TAG	UNP P68187
C	377	HIS	-	EXPRESSION TAG	UNP P68187
C	378	HIS	-	EXPRESSION TAG	UNP P68187
C	379	HIS	-	EXPRESSION TAG	UNP P68187
C	380	HIS	-	EXPRESSION TAG	UNP P68187
C	381	HIS	-	EXPRESSION TAG	UNP P68187
D	372	GLU	-	EXPRESSION TAG	UNP P68187
D	373	SER	-	EXPRESSION TAG	UNP P68187
D	374	ALA	-	EXPRESSION TAG	UNP P68187
D	375	SER	-	EXPRESSION TAG	UNP P68187
D	376	HIS	-	EXPRESSION TAG	UNP P68187
D	377	HIS	-	EXPRESSION TAG	UNP P68187
D	378	HIS	-	EXPRESSION TAG	UNP P68187
D	379	HIS	-	EXPRESSION TAG	UNP P68187
D	380	HIS	-	EXPRESSION TAG	UNP P68187
D	381	HIS	-	EXPRESSION TAG	UNP P68187

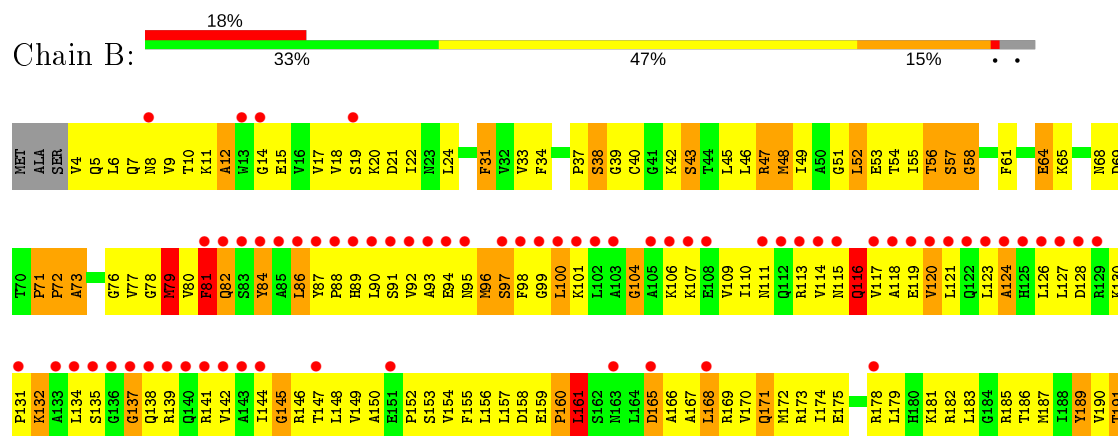
3 Residue-property plots

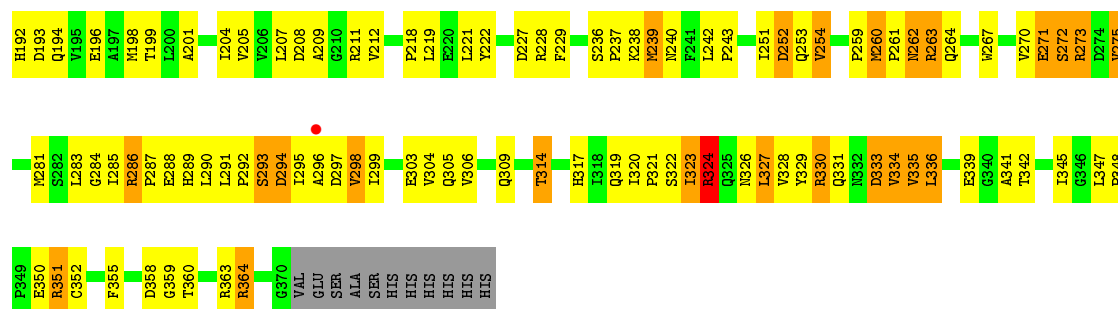
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Maltose/maltodextrin transport ATP-binding protein malK



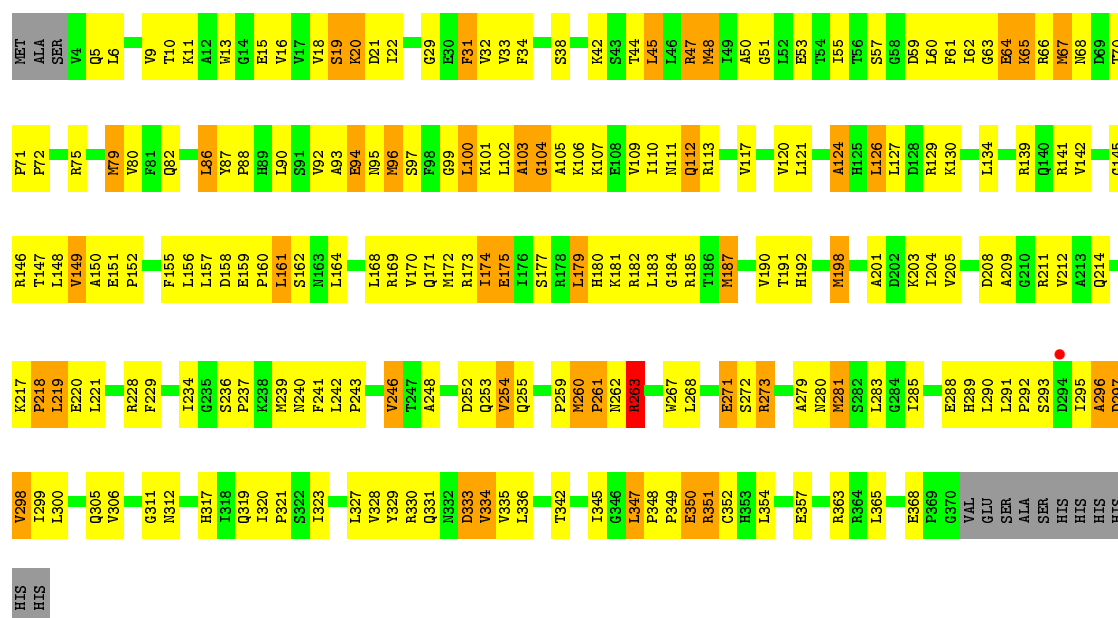
- Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK





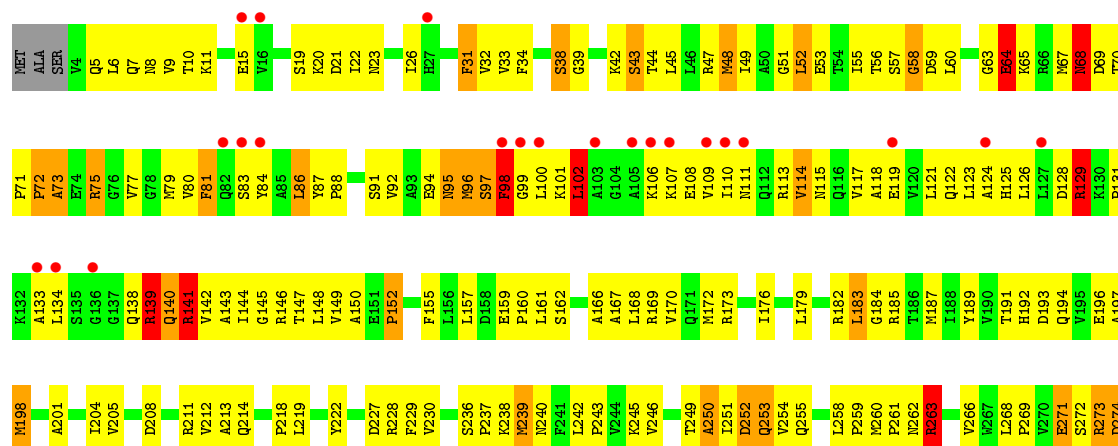
- Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK

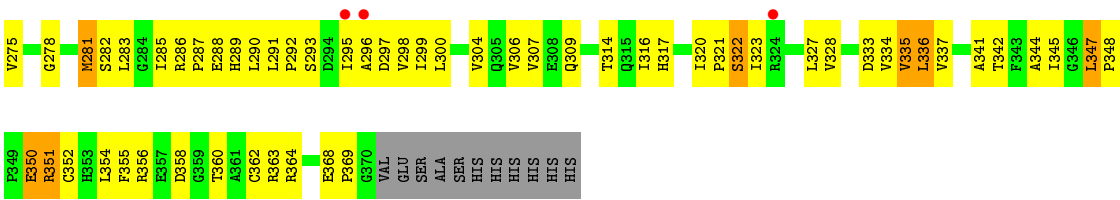
Chain C: 42% 43% 11%



- Molecule 1: Maltose/maltodextrin transport ATP-binding protein malK

Chain D: 7% 35% 50% 9%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.62Å 93.54Å 99.80Å 77.63° 79.38° 73.20°	Depositor
Resolution (Å)	15.54 – 2.80 15.54 – 2.73	Depositor EDS
% Data completeness (in resolution range)	92.5 (15.54-2.80) 89.5 (15.54-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.81 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.304 0.257 , 0.305	Depositor DCC
R_{free} test set	2445 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11412	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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	0.53	0/2903	0.86	7/3936 (0.2%)
1	B	0.52	0/2903	0.85	10/3936 (0.3%)
1	C	0.48	0/2903	0.84	12/3936 (0.3%)
1	D	0.45	0/2903	0.81	10/3936 (0.3%)
All	All	0.50	0/11612	0.84	39/15744 (0.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	C	66	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	A	169	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	D	169	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	D	141	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	B	363	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	B	330	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	D	139	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	C	47	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	C	263	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	B	364	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	D	263	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	B	47	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	B	324	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	324	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	286	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	C	334	VAL	CB-CA-C	-6.32	99.39	111.40
1	B	79	MET	CG-SD-CE	6.31	110.30	100.20
1	D	47	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	198	MET	CG-SD-CE	6.28	110.25	100.20
1	A	239	MET	CG-SD-CE	6.12	110.00	100.20
1	D	96	MET	CG-SD-CE	6.12	109.99	100.20
1	C	96	MET	CG-SD-CE	6.11	109.98	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	MET	CG-SD-CE	6.10	109.96	100.20
1	A	96	MET	CG-SD-CE	6.08	109.93	100.20
1	C	48	MET	CG-SD-CE	6.06	109.90	100.20
1	C	67	MET	CG-SD-CE	6.05	109.89	100.20
1	C	187	MET	CG-SD-CE	5.84	109.55	100.20
1	D	239	MET	CG-SD-CE	5.83	109.53	100.20
1	B	239	MET	CG-SD-CE	5.82	109.51	100.20
1	C	239	MET	CG-SD-CE	5.82	109.51	100.20
1	B	48	MET	CG-SD-CE	5.80	109.48	100.20
1	D	48	MET	CG-SD-CE	5.80	109.47	100.20
1	C	281	MET	CG-SD-CE	5.79	109.47	100.20
1	D	281	MET	CG-SD-CE	5.79	109.47	100.20
1	D	198	MET	CG-SD-CE	5.74	109.38	100.20
1	C	79	MET	CG-SD-CE	5.73	109.36	100.20
1	C	198	MET	CG-SD-CE	5.73	109.36	100.20
1	A	236	SER	O-C-N	-5.54	110.56	121.10

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	2853	0	2918	225	0
1	B	2853	0	2918	332	0
1	C	2853	0	2918	252	0
1	D	2853	0	2918	274	0
All	All	11412	0	11672	1075	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 47.

All (1075) 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:281:MET:CE	1:C:354:LEU:HD21	1.72	1.20
1:A:45:LEU:HD23	1:A:48:MET:CE	1.75	1.15
1:A:180:HIS:CG	1:A:187:MET:HE2	1.85	1.12
1:A:180:HIS:HB2	1:A:187:MET:CE	1.77	1.12
1:B:96:MET:HA	1:B:146:ARG:HA	1.18	1.12
1:C:180:HIS:HB2	1:C:187:MET:CE	1.79	1.11
1:C:281:MET:HE3	1:C:354:LEU:CD2	1.81	1.09
1:B:275:VAL:HG23	1:B:281:MET:HE3	1.35	1.08
1:A:90:LEU:HG	1:A:94:GLU:HG2	1.33	1.07
1:A:180:HIS:ND1	1:A:187:MET:HE2	1.69	1.07
1:A:45:LEU:HD23	1:A:48:MET:HE3	1.35	1.06
1:C:334:VAL:O	1:C:334:VAL:HG23	1.56	1.06
1:D:252:ASP:O	1:D:252:ASP:OD2	1.73	1.05
1:A:45:LEU:HA	1:A:48:MET:HE3	1.34	1.05
1:C:198:MET:HE3	1:C:218:PRO:HB3	1.34	1.04
1:B:120:VAL:HG21	1:B:175:GLU:HG3	1.37	1.03
1:C:180:HIS:CB	1:C:187:MET:HE2	1.88	1.03
1:A:180:HIS:CB	1:A:187:MET:HE2	1.88	1.03
1:A:180:HIS:HB2	1:A:187:MET:HE1	1.35	1.01
1:B:117:VAL:HG11	1:B:148:LEU:HD23	1.45	0.99
1:C:180:HIS:HB2	1:C:187:MET:HE2	1.44	0.98
1:A:132:LYS:HG2	1:A:133:ALA:H	1.30	0.97
1:C:290:LEU:HD13	1:C:345:ILE:HD12	1.47	0.96
1:C:45:LEU:HD23	1:C:48:MET:HE3	1.47	0.96
1:A:180:HIS:CG	1:A:187:MET:CE	2.48	0.95
1:A:180:HIS:CB	1:A:187:MET:CE	2.43	0.95
1:C:180:HIS:HB2	1:C:187:MET:HE1	1.48	0.95
1:D:87:TYR:HE2	1:D:98:PHE:CD2	1.84	0.95
1:B:130:LYS:H	1:B:130:LYS:HD2	1.32	0.94
1:B:275:VAL:HG23	1:B:281:MET:CE	1.97	0.94
1:B:45:LEU:HA	1:B:48:MET:HE3	1.50	0.94
1:D:173:ARG:HE	1:D:196:GLU:HG3	1.32	0.94
1:D:170:VAL:HA	1:D:173:ARG:NH1	1.84	0.93
1:C:198:MET:HE3	1:C:218:PRO:CB	1.99	0.93
1:B:92:VAL:HG23	1:B:131:PRO:HD3	1.47	0.93
1:D:170:VAL:HA	1:D:173:ARG:HH12	1.31	0.93
1:C:180:HIS:CG	1:C:187:MET:HE2	2.04	0.93
1:C:67:MET:CE	1:C:75:ARG:HA	1.99	0.92
1:C:170:VAL:HA	1:C:173:ARG:HH11	1.35	0.91
1:B:100:LEU:HD11	1:B:113:ARG:HD2	1.53	0.91
1:C:198:MET:CE	1:C:218:PRO:HB3	2.00	0.90
1:C:183:LEU:HD23	1:C:185:ARG:HE	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LEU:H	1:D:68:ASN:HD21	1.19	0.90
1:A:236:SER:O	1:A:238:LYS:N	2.05	0.90
1:B:334:VAL:HG23	1:B:335:VAL:H	1.37	0.89
1:D:87:TYR:HH	1:D:98:PHE:HE2	0.95	0.89
1:B:336:LEU:HD12	1:B:336:LEU:H	1.38	0.89
1:C:240:ASN:HD21	1:C:328:VAL:H	1.19	0.89
1:D:140:GLN:HA	1:D:143:ALA:HB3	1.55	0.89
1:C:297:ASP:O	1:C:298:VAL:HG23	1.73	0.89
1:B:168:LEU:HD23	1:B:171:GLN:HE22	1.37	0.88
1:D:290:LEU:HD13	1:D:345:ILE:HD12	1.54	0.88
1:D:289:HIS:ND1	1:D:351:ARG:HG2	1.87	0.88
1:A:205:VAL:HG23	1:A:215:VAL:HG22	1.52	0.88
1:D:336:LEU:HD12	1:D:336:LEU:H	1.36	0.88
1:D:68:ASN:H	1:D:68:ASN:HD22	1.13	0.88
1:B:254:VAL:HG23	1:B:272:SER:HB2	1.56	0.88
1:C:67:MET:HE2	1:C:75:ARG:HA	1.56	0.86
1:D:240:ASN:HD21	1:D:328:VAL:H	1.23	0.86
1:A:180:HIS:ND1	1:A:187:MET:CE	2.39	0.86
1:C:334:VAL:O	1:C:334:VAL:CG2	2.24	0.85
1:C:170:VAL:HA	1:C:173:ARG:NH1	1.91	0.85
1:A:45:LEU:HD23	1:A:48:MET:HE1	1.57	0.85
1:B:182:ARG:HG3	1:B:183:LEU:H	1.42	0.84
1:D:87:TYR:CE2	1:D:98:PHE:CD2	2.65	0.84
1:D:243:PRO:O	1:D:259:PRO:HG3	1.78	0.84
1:B:45:LEU:HA	1:B:48:MET:CE	2.08	0.84
1:C:22:ILE:HD12	1:C:45:LEU:HD11	1.58	0.84
1:D:87:TYR:OH	1:D:98:PHE:CE2	2.30	0.83
1:B:79:MET:HB2	1:B:156:LEU:HB2	1.59	0.83
1:A:148:LEU:HG	1:A:179:LEU:CD1	2.09	0.83
1:B:100:LEU:HD11	1:B:113:ARG:CD	2.08	0.83
1:B:114:VAL:HA	1:B:149:VAL:HG21	1.58	0.83
1:B:287:PRO:HB2	1:B:330:ARG:HG3	1.59	0.83
1:B:92:VAL:HA	1:B:95:ASN:HD22	1.41	0.82
1:C:198:MET:HE1	1:C:218:PRO:C	1.98	0.82
1:D:114:VAL:HG22	1:D:149:VAL:HG11	1.60	0.82
1:B:123:LEU:HD21	1:B:141:ARG:HG2	1.61	0.82
1:C:99:GLY:O	1:C:102:LEU:HB2	1.79	0.82
1:C:252:ASP:HB2	1:C:365:LEU:CD1	2.10	0.82
1:B:161:LEU:HB2	1:B:169:ARG:HG3	1.60	0.82
1:B:88:PRO:HB3	1:B:132:LYS:HD3	1.61	0.82
1:D:272:SER:O	1:D:275:VAL:HG12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:CD1	1:B:348:PRO:HG3	2.11	0.81
1:B:253:GLN:O	1:B:254:VAL:HB	1.78	0.81
1:A:63:GLY:O	1:A:64:GLU:HB2	1.81	0.81
1:B:81:PHE:HE1	1:B:84:TYR:HA	1.45	0.81
1:D:296:ALA:O	1:D:297:ASP:OD1	1.98	0.81
1:B:161:LEU:H	1:B:161:LEU:HD23	1.44	0.80
1:D:139:ARG:O	1:D:140:GLN:HG2	1.80	0.80
1:D:86:LEU:HD12	1:D:86:LEU:H	1.47	0.80
1:C:180:HIS:CB	1:C:187:MET:CE	2.53	0.80
1:C:312:ASN:HB2	1:D:288:GLU:HG2	1.64	0.80
1:D:252:ASP:OD2	1:D:252:ASP:C	2.20	0.79
1:A:237:PRO:HG2	1:A:330:ARG:HD2	1.64	0.79
1:C:105:ALA:HB3	1:C:109:VAL:HG21	1.65	0.79
1:C:121:LEU:HD22	1:C:172:MET:HE1	1.63	0.79
1:D:126:LEU:HD22	1:D:129:ARG:HD2	1.65	0.79
1:B:286:ARG:HB3	1:B:288:GLU:OE2	1.82	0.79
1:D:245:LYS:HE2	1:D:278:GLY:HA2	1.65	0.78
1:C:20:LYS:HE2	1:C:209:ALA:O	1.83	0.78
1:A:110:ILE:O	1:A:114:VAL:HG23	1.84	0.78
1:B:275:VAL:CG2	1:B:281:MET:HE3	2.11	0.78
1:C:100:LEU:C	1:C:102:LEU:H	1.85	0.78
1:D:281:MET:CE	1:D:354:LEU:HD21	2.13	0.77
1:B:253:GLN:HB3	1:B:267:TRP:HE3	1.50	0.77
1:D:87:TYR:OH	1:D:98:PHE:HE2	1.64	0.77
1:C:281:MET:HE3	1:C:354:LEU:HD21	0.86	0.77
1:D:252:ASP:O	1:D:253:GLN:HG3	1.84	0.77
1:D:68:ASN:N	1:D:68:ASN:HD22	1.82	0.77
1:D:297:ASP:O	1:D:299:ILE:HG13	1.83	0.77
1:B:275:VAL:CG2	1:B:281:MET:CE	2.62	0.77
1:A:95:ASN:O	1:A:96:MET:HB2	1.84	0.77
1:B:208:ASP:HB2	1:B:229:PHE:CZ	2.20	0.77
1:D:10:THR:HB	1:D:57:SER:HB3	1.66	0.76
1:B:109:VAL:HG23	1:B:110:ILE:HG13	1.67	0.76
1:C:327:LEU:HD23	1:C:345:ILE:HD11	1.65	0.76
1:A:236:SER:HB3	1:A:237:PRO:HD3	1.67	0.76
1:B:34:PHE:HE1	1:B:45:LEU:HD22	1.51	0.76
1:D:183:LEU:O	1:D:185:ARG:HG2	1.85	0.76
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.50	0.76
1:D:11:LYS:HB2	1:D:48:MET:SD	2.25	0.75
1:A:334:VAL:HG23	1:A:334:VAL:O	1.84	0.75
1:A:90:LEU:HG	1:A:94:GLU:CG	2.13	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LYS:HG2	1:B:211:ARG:CZ	2.16	0.75
1:C:80:VAL:HG12	1:C:157:LEU:HD22	1.68	0.75
1:C:10:THR:HB	1:C:57:SER:HB3	1.68	0.75
1:C:180:HIS:ND1	1:C:187:MET:HE2	2.00	0.75
1:C:95:ASN:O	1:C:96:MET:HB3	1.87	0.75
1:D:97:SER:O	1:D:99:GLY:N	2.20	0.75
1:B:118:ALA:HB1	1:B:123:LEU:HB3	1.66	0.74
1:B:275:VAL:HB	1:B:281:MET:HE1	1.69	0.74
1:D:281:MET:HE1	1:D:354:LEU:HD21	1.68	0.74
1:C:31:PHE:CD2	1:C:187:MET:HE3	2.22	0.74
1:B:79:MET:O	1:B:79:MET:HG2	1.86	0.74
1:B:253:GLN:HB3	1:B:267:TRP:CE3	2.23	0.74
1:B:34:PHE:HB2	1:B:190:VAL:HG22	1.70	0.73
1:D:100:LEU:HD12	1:D:113:ARG:HH22	1.53	0.73
1:C:80:VAL:HG12	1:C:157:LEU:CD2	2.18	0.73
1:B:251:ILE:O	1:B:252:ASP:HB3	1.88	0.73
1:C:180:HIS:CG	1:C:187:MET:CE	2.70	0.73
1:B:86:LEU:HD21	1:B:139:ARG:HB3	1.69	0.73
1:C:214:GLN:HG2	1:C:221:LEU:CD2	2.19	0.73
1:B:78:GLY:O	1:B:79:MET:HB3	1.89	0.73
1:C:45:LEU:CD2	1:C:48:MET:HE3	2.18	0.73
1:B:100:LEU:HD22	1:B:109:VAL:HB	1.69	0.72
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.53	0.72
1:D:252:ASP:O	1:D:252:ASP:CG	2.25	0.72
1:C:100:LEU:O	1:C:102:LEU:N	2.22	0.72
1:B:161:LEU:HD13	1:B:172:MET:HB2	1.71	0.72
1:D:80:VAL:HG21	1:D:144:ILE:HA	1.70	0.72
1:B:80:VAL:HG11	1:B:144:ILE:O	1.89	0.72
1:A:291:LEU:HG	1:A:348:PRO:HG3	1.72	0.72
1:A:321:PRO:O	1:A:322:SER:OG	2.08	0.72
1:B:45:LEU:O	1:B:49:ILE:HG13	1.89	0.72
1:C:334:VAL:HG21	1:D:369:PRO:HG2	1.70	0.72
1:C:214:GLN:HG2	1:C:221:LEU:HD21	1.71	0.72
1:D:126:LEU:HD11	1:D:138:GLN:NE2	2.04	0.72
1:C:45:LEU:HD23	1:C:48:MET:CE	2.19	0.71
1:C:96:MET:HA	1:C:146:ARG:HA	1.71	0.71
1:D:194:GLN:O	1:D:198:MET:HG2	1.90	0.71
1:C:100:LEU:C	1:C:102:LEU:N	2.41	0.71
1:D:64:GLU:OE1	1:D:64:GLU:HA	1.90	0.71
1:B:309:GLN:NE2	1:B:314:THR:CG2	2.53	0.71
1:C:164:LEU:HD22	1:C:168:LEU:HD22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:CD2	1:A:48:MET:HE3	2.19	0.71
1:C:198:MET:CE	1:C:218:PRO:CB	2.64	0.71
1:D:99:GLY:O	1:D:100:LEU:HD22	1.91	0.71
1:B:290:LEU:HD13	1:B:345:ILE:HD12	1.74	0.70
1:A:100:LEU:HB2	1:A:150:ALA:HA	1.73	0.70
1:B:171:GLN:O	1:B:175:GLU:HG2	1.91	0.70
1:C:47:ARG:HB3	1:C:53:GLU:HG2	1.72	0.70
1:B:20:LYS:HG2	1:B:211:ARG:NH1	2.05	0.70
1:B:47:ARG:HB3	1:B:52:LEU:HB2	1.73	0.70
1:D:101:LYS:HA	1:D:109:VAL:HG21	1.73	0.70
1:A:286:ARG:HB3	1:A:288:GLU:OE2	1.92	0.70
1:D:117:VAL:HG12	1:D:148:LEU:HD23	1.73	0.70
1:D:8:ASN:H	1:D:23:ASN:ND2	1.90	0.70
1:C:236:SER:HA	1:C:237:PRO:C	2.12	0.70
1:A:6:LEU:HD23	1:A:22:ILE:HD11	1.74	0.70
1:A:166:ALA:O	1:A:167:ALA:CB	2.39	0.69
1:D:240:ASN:ND2	1:D:328:VAL:H	1.90	0.69
1:D:320:ILE:HD11	1:D:327:LEU:HD22	1.73	0.69
1:B:171:GLN:HG2	1:B:172:MET:N	2.06	0.69
1:C:60:LEU:H	1:C:68:ASN:HD21	1.38	0.69
1:A:132:LYS:HG2	1:A:133:ALA:N	2.05	0.69
1:C:22:ILE:CD1	1:C:45:LEU:HD11	2.22	0.69
1:D:159:GLU:N	1:D:160:PRO:HD3	2.06	0.69
1:A:34:PHE:CD2	1:A:205:VAL:CG1	2.76	0.69
1:B:126:LEU:HD11	1:B:138:GLN:CD	2.13	0.69
1:A:45:LEU:HA	1:A:48:MET:CE	2.18	0.69
1:D:140:GLN:HA	1:D:143:ALA:CB	2.23	0.69
1:C:31:PHE:CD2	1:C:187:MET:CE	2.76	0.68
1:D:92:VAL:HG21	1:D:126:LEU:O	1.93	0.68
1:D:292:PRO:O	1:D:293:SER:HB3	1.92	0.68
1:A:166:ALA:O	1:A:167:ALA:HB3	1.93	0.68
1:D:139:ARG:HG2	1:D:140:GLN:H	1.58	0.68
1:B:168:LEU:HD23	1:B:171:GLN:NE2	2.08	0.68
1:C:228:ARG:HH11	1:C:228:ARG:HG2	1.57	0.68
1:B:126:LEU:HD11	1:B:138:GLN:OE1	1.93	0.68
1:D:117:VAL:HG22	1:D:182:ARG:HH12	1.57	0.68
1:C:271:GLU:HG3	1:C:273:ARG:HB2	1.75	0.68
1:A:177:SER:O	1:A:181:LYS:HG2	1.94	0.68
1:A:66:ARG:NH1	1:A:68:ASN:HB2	2.08	0.68
1:C:240:ASN:HD21	1:C:328:VAL:N	1.91	0.68
1:C:280:ASN:O	1:C:357:GLU:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:CD1	1:D:142:VAL:HG22	2.23	0.68
1:D:290:LEU:HD13	1:D:345:ILE:CD1	2.22	0.68
1:D:242:LEU:HD12	1:D:283:LEU:HD22	1.74	0.67
1:A:98:PHE:O	1:A:101:LYS:HB3	1.94	0.67
1:A:31:PHE:CD2	1:A:187:MET:HE3	2.30	0.67
1:B:6:LEU:O	1:B:7:GLN:HG3	1.94	0.67
1:A:65:LYS:N	1:A:65:LYS:HD3	2.10	0.67
1:C:96:MET:CE	1:C:142:VAL:HA	2.25	0.67
1:D:236:SER:HA	1:D:237:PRO:C	2.15	0.67
1:A:132:LYS:O	1:A:133:ALA:C	2.33	0.67
1:D:351:ARG:HA	1:D:364:ARG:HH21	1.60	0.67
1:A:214:GLN:HG2	1:A:221:LEU:HD22	1.75	0.67
1:C:240:ASN:ND2	1:C:327:LEU:HA	2.10	0.67
1:C:63:GLY:O	1:C:64:GLU:HB2	1.94	0.67
1:C:183:LEU:HD23	1:C:185:ARG:NE	2.09	0.67
1:A:173:ARG:HE	1:A:196:GLU:HG3	1.57	0.66
1:B:86:LEU:CD2	1:B:139:ARG:HB3	2.24	0.66
1:D:123:LEU:HD13	1:D:142:VAL:HG22	1.76	0.66
1:B:126:LEU:HD21	1:B:138:GLN:NE2	2.10	0.66
1:B:145:GLY:HA2	1:B:148:LEU:HD13	1.75	0.66
1:B:159:GLU:N	1:B:160:PRO:HD3	2.09	0.66
1:D:68:ASN:ND2	1:D:68:ASN:H	1.90	0.66
1:B:243:PRO:O	1:B:259:PRO:HG3	1.95	0.66
1:B:33:VAL:HG23	1:B:201:ALA:HB2	1.75	0.66
1:B:56:THR:O	1:B:57:SER:HB2	1.94	0.66
1:B:80:VAL:HG13	1:B:84:TYR:CD1	2.29	0.66
1:D:271:GLU:O	1:D:272:SER:HB3	1.96	0.66
1:B:17:VAL:HG12	1:B:19:SER:H	1.59	0.66
1:B:45:LEU:O	1:B:45:LEU:HD23	1.96	0.66
1:D:126:LEU:CD2	1:D:129:ARG:HD2	2.24	0.66
1:D:307:VAL:HG12	1:D:309:GLN:HE21	1.60	0.66
1:C:42:LYS:HD2	1:C:190:VAL:HG13	1.77	0.66
1:B:189:TYR:HE2	1:B:191:THR:CG2	2.08	0.66
1:B:321:PRO:O	1:B:322:SER:OG	2.12	0.66
1:B:99:GLY:O	1:B:100:LEU:CB	2.44	0.66
1:C:148:LEU:HD22	1:C:179:LEU:HD13	1.78	0.66
1:C:243:PRO:O	1:C:259:PRO:HG3	1.96	0.66
1:D:60:LEU:N	1:D:68:ASN:HD21	1.89	0.65
1:A:252:ASP:HB2	1:A:365:LEU:CD1	2.26	0.65
1:B:189:TYR:HE2	1:B:191:THR:HG23	1.61	0.65
1:D:271:GLU:HG2	1:D:356:ARG:HH22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:O	1:B:111:ASN:HB2	1.97	0.65
1:A:132:LYS:CG	1:A:133:ALA:H	2.08	0.65
1:C:124:ALA:O	1:C:127:LEU:HD12	1.97	0.65
1:B:98:PHE:HA	1:B:101:LYS:HZ2	1.61	0.65
1:D:228:ARG:HH11	1:D:228:ARG:HG2	1.61	0.65
1:B:291:LEU:HD12	1:B:348:PRO:HG3	1.79	0.65
1:A:9:VAL:HB	1:A:22:ILE:HG12	1.78	0.64
1:C:62:ILE:HB	1:C:67:MET:HG3	1.78	0.64
1:A:105:ALA:HB3	1:A:109:VAL:HG21	1.79	0.64
1:B:116:GLN:O	1:B:119:GLU:HB2	1.97	0.64
1:A:297:ASP:O	1:A:298:VAL:HB	1.97	0.64
1:A:334:VAL:CG2	1:A:334:VAL:O	2.46	0.64
1:B:11:LYS:HB3	1:B:19:SER:HB2	1.77	0.64
1:C:297:ASP:O	1:C:298:VAL:CG2	2.46	0.64
1:C:106:LYS:O	1:C:109:VAL:HG22	1.97	0.64
1:B:101:LYS:HB3	1:B:101:LYS:NZ	2.12	0.64
1:B:79:MET:CG	1:B:79:MET:O	2.44	0.64
1:C:152:PRO:O	1:C:185:ARG:HD3	1.97	0.64
1:C:253:GLN:HB3	1:C:267:TRP:CE3	2.32	0.64
1:C:299:ILE:C	1:C:300:LEU:HD12	2.18	0.64
1:D:84:TYR:HB3	1:D:146:ARG:HH22	1.61	0.64
1:D:33:VAL:HG23	1:D:201:ALA:HB2	1.79	0.64
1:A:105:ALA:HB3	1:A:109:VAL:CG2	2.27	0.64
1:C:253:GLN:O	1:C:254:VAL:HB	1.98	0.64
1:A:308:GLU:HG2	1:B:199:THR:HG23	1.80	0.63
1:A:289:HIS:ND1	1:A:351:ARG:HG2	2.13	0.63
1:B:295:ILE:HD12	1:B:295:ILE:N	2.14	0.63
1:D:34:PHE:HE1	1:D:45:LEU:HD22	1.63	0.63
1:A:243:PRO:O	1:A:259:PRO:HG3	1.99	0.63
1:B:320:ILE:HG21	1:B:323:ILE:HD12	1.80	0.63
1:D:121:LEU:HD11	1:D:148:LEU:HD22	1.79	0.63
1:B:98:PHE:HE1	1:B:146:ARG:HH11	1.46	0.63
1:A:148:LEU:HG	1:A:179:LEU:HD11	1.78	0.63
1:D:144:ILE:O	1:D:148:LEU:N	2.31	0.63
1:A:76:GLY:O	1:A:153:SER:HB3	1.99	0.63
1:A:99:GLY:C	1:A:101:LYS:H	2.00	0.63
1:C:254:VAL:HG23	1:C:272:SER:HB2	1.80	0.63
1:D:295:ILE:HD12	1:D:295:ILE:N	2.14	0.63
1:B:183:LEU:C	1:B:185:ARG:H	2.02	0.63
1:C:102:LEU:O	1:C:103:ALA:HB2	1.99	0.63
1:D:139:ARG:HD3	1:D:140:GLN:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:LEU:HB3	1:D:95:ASN:OD1	1.99	0.63
1:A:242:LEU:O	1:A:244:VAL:HG13	1.99	0.62
1:A:253:GLN:O	1:A:254:VAL:HB	1.99	0.62
1:B:117:VAL:HG11	1:B:148:LEU:CD2	2.26	0.62
1:B:275:VAL:CB	1:B:281:MET:HE1	2.28	0.62
1:C:292:PRO:O	1:C:293:SER:HB3	1.98	0.62
1:B:142:VAL:HG12	1:B:142:VAL:O	1.99	0.62
1:A:329:TYR:CE2	1:A:331:GLN:HB2	2.34	0.62
1:C:159:GLU:OE2	1:C:191:THR:HG22	1.99	0.62
1:D:100:LEU:HD12	1:D:113:ARG:NH2	2.14	0.62
1:A:236:SER:HB3	1:A:237:PRO:CD	2.30	0.62
1:A:141:ARG:HG2	1:A:172:MET:CE	2.29	0.62
1:D:110:ILE:N	1:D:110:ILE:HD12	2.15	0.62
1:C:20:LYS:H	1:C:20:LYS:HD2	1.65	0.62
1:D:271:GLU:HG3	1:D:273:ARG:H	1.64	0.62
1:D:334:VAL:HG23	1:D:335:VAL:N	2.14	0.62
1:A:100:LEU:HG	1:A:100:LEU:O	1.98	0.62
1:B:161:LEU:N	1:B:161:LEU:HD23	2.14	0.62
1:B:306:VAL:HB	1:B:317:HIS:CG	2.35	0.62
1:B:92:VAL:HG22	1:B:142:VAL:HG11	1.81	0.62
1:D:211:ARG:HG3	1:D:212:VAL:H	1.64	0.62
1:A:369:PRO:HG2	1:B:334:VAL:HG11	1.81	0.62
1:D:101:LYS:O	1:D:102:LEU:C	2.37	0.62
1:D:152:PRO:HD2	1:D:155:PHE:HE2	1.65	0.62
1:D:271:GLU:HG2	1:D:356:ARG:NH2	2.15	0.62
1:A:22:ILE:HD11	1:A:45:LEU:HD21	1.80	0.61
1:C:121:LEU:HD22	1:C:172:MET:CE	2.30	0.61
1:C:298:VAL:CG1	1:C:347:LEU:HB3	2.30	0.61
1:C:198:MET:HE1	1:C:218:PRO:CA	2.30	0.61
1:D:334:VAL:HG23	1:D:335:VAL:H	1.65	0.61
1:A:261:PRO:O	1:A:263:ARG:N	2.33	0.61
1:A:122:GLN:HB2	1:A:141:ARG:HH21	1.65	0.61
1:A:253:GLN:HB3	1:A:267:TRP:CE3	2.35	0.61
1:D:101:LYS:O	1:D:102:LEU:O	2.18	0.61
1:D:107:LYS:HD2	1:D:107:LYS:C	2.21	0.61
1:B:168:LEU:HA	1:B:171:GLN:NE2	2.15	0.61
1:B:20:LYS:O	1:B:22:ILE:HG23	2.01	0.61
1:C:87:TYR:H	1:C:95:ASN:ND2	1.98	0.61
1:B:92:VAL:HB	1:B:128:ASP:C	2.21	0.61
1:B:288:GLU:HG3	1:B:330:ARG:HD3	1.81	0.61
1:B:145:GLY:HA2	1:B:148:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:VAL:CG2	1:B:281:MET:HE1	2.31	0.61
1:B:297:ASP:O	1:B:298:VAL:HB	2.00	0.61
1:B:90:LEU:HD23	1:B:94:GLU:HB3	1.80	0.61
1:C:347:LEU:O	1:C:349:PRO:HD3	2.01	0.61
1:D:289:HIS:ND1	1:D:351:ARG:CG	2.60	0.61
1:C:295:ILE:HD12	1:C:295:ILE:N	2.15	0.61
1:A:214:GLN:HG2	1:A:221:LEU:CD2	2.31	0.60
1:A:246:VAL:HG12	1:A:279:ALA:O	1.99	0.60
1:D:289:HIS:CG	1:D:351:ARG:HG2	2.36	0.60
1:B:182:ARG:HG3	1:B:183:LEU:N	2.13	0.60
1:C:47:ARG:NH1	1:C:53:GLU:OE2	2.32	0.60
1:A:62:ILE:C	1:A:64:GLU:H	2.05	0.60
1:C:9:VAL:HB	1:C:22:ILE:HG12	1.82	0.60
1:A:314:THR:HG22	1:A:316:ILE:HD11	1.83	0.60
1:B:207:LEU:HD21	1:B:212:VAL:HG22	1.82	0.60
1:B:51:GLY:O	1:B:53:GLU:N	2.34	0.60
1:D:347:LEU:HD21	1:D:352:CYS:SG	2.41	0.60
1:B:170:VAL:HA	1:B:173:ARG:HH12	1.66	0.60
1:B:154:VAL:HG12	1:B:186:THR:HB	1.83	0.60
1:C:331:GLN:CD	1:C:335:VAL:HG21	2.21	0.60
1:A:122:GLN:HB2	1:A:141:ARG:NH2	2.16	0.60
1:B:165:ASP:C	1:B:167:ALA:H	2.04	0.60
1:B:175:GLU:HB3	1:B:178:ARG:NH2	2.16	0.60
1:C:300:LEU:HD12	1:C:300:LEU:N	2.17	0.60
1:D:297:ASP:O	1:D:298:VAL:C	2.40	0.60
1:B:130:LYS:H	1:B:130:LYS:CD	2.10	0.60
1:D:291:LEU:HB3	1:D:292:PRO:HD2	1.83	0.60
1:A:42:LYS:NZ	1:A:192:HIS:NE2	2.48	0.60
1:A:217:LYS:O	1:A:220:GLU:HB2	2.02	0.60
1:B:110:ILE:HA	1:B:114:VAL:HB	1.83	0.60
1:A:64:GLU:HB3	1:A:65:LYS:HD3	1.83	0.60
1:D:336:LEU:CD1	1:D:336:LEU:H	2.14	0.60
1:B:80:VAL:HG13	1:B:84:TYR:HD1	1.67	0.59
1:B:6:LEU:HD23	1:B:9:VAL:HG21	1.84	0.59
1:C:67:MET:HE2	1:C:75:ARG:CA	2.31	0.59
1:B:292:PRO:O	1:B:294:ASP:N	2.30	0.59
1:D:358:ASP:HB3	1:D:360:THR:OG1	2.02	0.59
1:C:22:ILE:HD11	1:C:45:LEU:HD21	1.83	0.59
1:A:281:MET:CE	1:A:354:LEU:HD21	2.32	0.59
1:B:96:MET:HA	1:B:146:ARG:CA	2.12	0.59
1:C:156:LEU:O	1:C:157:LEU:HD23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:LEU:HD12	1:D:336:LEU:N	2.11	0.59
1:C:252:ASP:HB2	1:C:365:LEU:HD11	1.83	0.59
1:A:6:LEU:CD2	1:A:22:ILE:HD11	2.32	0.59
1:A:292:PRO:O	1:A:293:SER:CB	2.51	0.59
1:C:42:LYS:NZ	1:C:192:HIS:NE2	2.50	0.59
1:A:271:GLU:HB2	1:A:363:ARG:HB3	1.85	0.59
1:D:109:VAL:HB	1:D:110:ILE:HD12	1.85	0.59
1:D:152:PRO:HD2	1:D:155:PHE:CE2	2.37	0.59
1:A:130:LYS:HG3	1:A:131:PRO:HD2	1.85	0.59
1:B:155:PHE:O	1:B:156:LEU:HD23	2.03	0.59
1:B:194:GLN:O	1:B:198:MET:HG2	2.02	0.59
1:C:148:LEU:HD23	1:C:155:PHE:CE2	2.38	0.59
1:C:248:ALA:HB3	1:C:255:GLN:HE21	1.66	0.59
1:D:240:ASN:HD21	1:D:328:VAL:N	1.97	0.59
1:A:159:GLU:N	1:A:160:PRO:HD3	2.16	0.58
1:B:296:ALA:HA	1:B:299:ILE:HD11	1.83	0.58
1:C:342:THR:HG23	1:C:342:THR:O	2.02	0.58
1:B:171:GLN:O	1:B:174:ILE:HB	2.02	0.58
1:C:60:LEU:N	1:C:68:ASN:HD21	1.99	0.58
1:D:272:SER:O	1:D:273:ARG:O	2.21	0.58
1:A:120:VAL:HG13	1:A:175:GLU:OE1	2.02	0.58
1:B:113:ARG:O	1:B:149:VAL:HG11	2.03	0.58
1:B:117:VAL:C	1:B:119:GLU:H	2.07	0.58
1:B:96:MET:HG2	1:B:145:GLY:C	2.24	0.58
1:D:252:ASP:O	1:D:253:GLN:CB	2.50	0.58
1:A:42:LYS:HZ1	1:A:192:HIS:CE1	2.22	0.58
1:B:253:GLN:O	1:B:254:VAL:CB	2.51	0.58
1:B:160:PRO:HB2	1:B:161:LEU:HD23	1.85	0.58
1:B:350:GLU:CD	1:B:350:GLU:H	2.06	0.58
1:C:145:GLY:O	1:C:149:VAL:HG13	2.02	0.58
1:C:253:GLN:HB3	1:C:267:TRP:HE3	1.66	0.58
1:C:351:ARG:HD2	1:C:368:GLU:OE2	2.03	0.58
1:C:22:ILE:CD1	1:C:45:LEU:HD21	2.34	0.58
1:D:306:VAL:HB	1:D:317:HIS:HB2	1.85	0.58
1:B:92:VAL:CG2	1:B:131:PRO:HD3	2.27	0.58
1:B:309:GLN:HE22	1:B:314:THR:HG21	1.69	0.57
1:B:93:ALA:HA	1:B:128:ASP:OD1	2.04	0.57
1:A:17:VAL:HG11	1:A:20:LYS:HG2	1.84	0.57
1:A:34:PHE:CD2	1:A:205:VAL:HG12	2.39	0.57
1:A:66:ARG:HH12	1:A:68:ASN:HB2	1.68	0.57
1:B:123:LEU:HD21	1:B:141:ARG:CG	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:SER:OG	1:B:39:GLY:N	2.37	0.57
1:A:159:GLU:HG3	1:A:162:SER:HB2	1.85	0.57
1:A:281:MET:HE1	1:A:354:LEU:HD21	1.85	0.57
1:D:98:PHE:CD1	1:D:98:PHE:C	2.77	0.57
1:A:132:LYS:O	1:A:134:LEU:N	2.37	0.57
1:B:86:LEU:HD12	1:B:86:LEU:H	1.70	0.57
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.70	0.57
1:B:314:THR:HG21	1:B:334:VAL:O	2.05	0.57
1:B:12:ALA:HB2	1:B:17:VAL:HA	1.85	0.57
1:B:199:THR:HG22	1:B:199:THR:O	2.04	0.57
1:D:157:LEU:HB3	1:D:160:PRO:HG3	1.86	0.57
1:B:87:TYR:CE2	1:B:98:PHE:CZ	2.93	0.57
1:B:99:GLY:O	1:B:100:LEU:HB2	2.05	0.57
1:C:34:PHE:HB2	1:C:190:VAL:HG22	1.86	0.57
1:D:155:PHE:HB2	1:D:187:MET:HG2	1.87	0.57
1:C:174:ILE:O	1:C:177:SER:N	2.38	0.57
1:B:131:PRO:HA	1:B:134:LEU:CD1	2.34	0.57
1:B:309:GLN:NE2	1:B:314:THR:HG21	2.19	0.57
1:B:92:VAL:HG23	1:B:131:PRO:CD	2.31	0.57
1:D:291:LEU:CD1	1:D:348:PRO:HG3	2.35	0.57
1:A:141:ARG:HG2	1:A:172:MET:HE3	1.87	0.56
1:A:211:ARG:HG3	1:A:212:VAL:H	1.70	0.56
1:A:289:HIS:O	1:A:348:PRO:HG2	2.04	0.56
1:B:104:GLY:HA3	1:B:109:VAL:HG11	1.87	0.56
1:B:251:ILE:O	1:B:252:ASP:CB	2.53	0.56
1:B:98:PHE:HA	1:B:101:LYS:NZ	2.21	0.56
1:D:261:PRO:O	1:D:262:ASN:CG	2.42	0.56
1:A:99:GLY:O	1:A:100:LEU:HB3	2.06	0.56
1:A:31:PHE:CD2	1:A:187:MET:CE	2.89	0.56
1:C:141:ARG:HD2	1:C:168:LEU:HD21	1.88	0.56
1:D:182:ARG:HB3	1:D:183:LEU:HD23	1.85	0.56
1:C:20:LYS:CD	1:C:20:LYS:H	2.19	0.56
1:C:327:LEU:CD2	1:C:345:ILE:HD11	2.35	0.56
1:C:347:LEU:HD21	1:C:352:CYS:SG	2.44	0.56
1:B:207:LEU:HD23	1:B:212:VAL:HA	1.88	0.56
1:B:264:GLN:OE1	1:B:298:VAL:HG22	2.05	0.56
1:D:252:ASP:O	1:D:253:GLN:CG	2.51	0.56
1:A:102:LEU:O	1:A:103:ALA:CB	2.53	0.56
1:A:240:ASN:HD21	1:A:328:VAL:H	1.52	0.56
1:C:291:LEU:HG	1:C:348:PRO:HG3	1.88	0.56
1:D:327:LEU:HD23	1:D:345:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:N	1:A:220:GLU:OE1	2.29	0.56
1:D:107:LYS:HD2	1:D:107:LYS:O	2.05	0.56
1:D:139:ARG:C	1:D:141:ARG:H	2.09	0.56
1:C:347:LEU:CD2	1:C:352:CYS:SG	2.94	0.56
1:D:96:MET:CE	1:D:121:LEU:HD12	2.36	0.56
1:B:334:VAL:HG23	1:B:335:VAL:N	2.15	0.56
1:C:164:LEU:HD22	1:C:168:LEU:CD2	2.36	0.56
1:C:59:ASP:HB3	1:C:61:PHE:CE1	2.40	0.56
1:C:126:LEU:HD22	1:C:134:LEU:HD22	1.88	0.56
1:D:285:ILE:HG12	1:D:290:LEU:HD23	1.88	0.56
1:C:201:ALA:HB1	1:C:203:LYS:O	2.07	0.55
1:C:289:HIS:ND1	1:C:351:ARG:HG2	2.20	0.55
1:C:87:TYR:H	1:C:95:ASN:HD21	1.53	0.55
1:D:96:MET:HE3	1:D:145:GLY:HA3	1.88	0.55
1:D:96:MET:CE	1:D:145:GLY:HA3	2.35	0.55
1:A:331:GLN:OE1	1:A:335:VAL:HG22	2.06	0.55
1:B:303:GLU:HA	1:B:341:ALA:O	2.06	0.55
1:D:114:VAL:O	1:D:118:ALA:HB2	2.07	0.55
1:D:327:LEU:CD2	1:D:345:ILE:HD11	2.36	0.55
1:A:34:PHE:HD2	1:A:205:VAL:HG12	1.71	0.55
1:A:271:GLU:OE1	1:A:363:ARG:HB3	2.07	0.55
1:A:89:HIS:NE2	1:A:90:LEU:HD13	2.22	0.55
1:D:11:LYS:HB3	1:D:19:SER:HB3	1.88	0.55
1:C:96:MET:HE2	1:C:142:VAL:HG13	1.89	0.55
1:C:96:MET:HE2	1:C:142:VAL:HA	1.88	0.55
1:B:251:ILE:HG22	1:B:251:ILE:O	2.06	0.55
1:A:10:THR:HB	1:A:57:SER:HB3	1.88	0.55
1:B:165:ASP:O	1:B:167:ALA:N	2.31	0.55
1:C:179:LEU:HG	1:C:183:LEU:HD13	1.88	0.55
1:C:198:MET:CE	1:C:218:PRO:CA	2.84	0.55
1:C:288:GLU:HG3	1:C:330:ARG:HD3	1.87	0.55
1:D:281:MET:HE3	1:D:354:LEU:HD21	1.88	0.55
1:C:255:GLN:HB2	1:C:267:TRP:CD2	2.42	0.55
1:D:108:GLU:HA	1:D:111:ASN:HB3	1.89	0.55
1:A:97:SER:O	1:A:101:LYS:HB2	2.06	0.55
1:D:183:LEU:O	1:D:185:ARG:N	2.39	0.55
1:B:293:SER:C	1:B:295:ILE:H	2.10	0.55
1:D:55:ILE:HG22	1:D:57:SER:O	2.06	0.55
1:A:253:GLN:O	1:A:268:LEU:O	2.24	0.54
1:B:261:PRO:O	1:B:263:ARG:N	2.41	0.54
1:D:251:ILE:O	1:D:252:ASP:CG	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ILE:HG12	1:D:290:LEU:CD2	2.36	0.54
1:B:10:THR:HB	1:B:57:SER:HB3	1.87	0.54
1:C:96:MET:HA	1:C:146:ARG:CA	2.38	0.54
1:D:260:MET:HA	1:D:322:SER:OG	2.07	0.54
1:B:22:ILE:HD12	1:B:24:LEU:HD13	1.88	0.54
1:B:254:VAL:CG2	1:B:272:SER:HB2	2.35	0.54
1:B:91:SER:OG	1:B:130:LYS:HG3	2.08	0.54
1:B:252:ASP:O	1:B:253:GLN:HG2	2.07	0.54
1:C:320:ILE:HB	1:C:323:ILE:HD12	1.90	0.54
1:C:312:ASN:CB	1:D:288:GLU:HG2	2.34	0.54
1:B:100:LEU:HD11	1:B:113:ARG:HD3	1.86	0.54
1:B:98:PHE:HE1	1:B:146:ARG:NH1	2.04	0.54
1:D:320:ILE:HB	1:D:323:ILE:HD12	1.90	0.54
1:A:5:GLN:C	1:A:6:LEU:HD12	2.28	0.54
1:C:102:LEU:O	1:C:103:ALA:CB	2.56	0.54
1:C:180:HIS:ND1	1:C:187:MET:CE	2.69	0.54
1:D:139:ARG:HG2	1:D:140:GLN:N	2.22	0.54
1:A:329:TYR:HE2	1:A:331:GLN:HB2	1.72	0.54
1:B:7:GLN:O	1:B:9:VAL:N	2.41	0.54
1:B:97:SER:OG	1:B:98:PHE:N	2.38	0.54
1:D:110:ILE:HG22	1:D:110:ILE:O	2.08	0.54
1:D:117:VAL:O	1:D:117:VAL:HG12	2.08	0.54
1:D:80:VAL:HG23	1:D:143:ALA:O	2.08	0.54
1:B:305:GLN:CD	1:B:319:GLN:HB2	2.28	0.54
1:C:86:LEU:O	1:C:88:PRO:HD3	2.08	0.54
1:A:180:HIS:CB	1:A:187:MET:HE1	2.18	0.53
1:B:110:ILE:O	1:B:110:ILE:HG22	2.08	0.53
1:C:198:MET:HE1	1:C:218:PRO:O	2.07	0.53
1:B:170:VAL:HA	1:B:173:ARG:NH1	2.23	0.53
1:C:6:LEU:HD23	1:C:22:ILE:HD11	1.90	0.53
1:D:126:LEU:HD11	1:D:138:GLN:CD	2.28	0.53
1:A:112:GLN:HG3	1:A:113:ARG:N	2.24	0.53
1:A:59:ASP:HB3	1:A:61:PHE:CE1	2.44	0.53
1:B:236:SER:HA	1:B:237:PRO:C	2.27	0.53
1:C:261:PRO:C	1:C:263:ARG:H	2.12	0.53
1:D:121:LEU:O	1:D:141:ARG:NH1	2.42	0.53
1:D:263:ARG:HH11	1:D:263:ARG:HG2	1.73	0.53
1:A:178:ARG:HG3	1:A:178:ARG:NH1	2.21	0.53
1:C:148:LEU:HD22	1:C:179:LEU:CD1	2.37	0.53
1:C:90:LEU:HG	1:C:94:GLU:HB3	1.90	0.53
1:D:86:LEU:O	1:D:88:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:CD2	1:B:49:ILE:HD11	2.39	0.53
1:B:64:GLU:OE1	1:B:64:GLU:HA	2.08	0.53
1:C:255:GLN:HB2	1:C:267:TRP:CE2	2.44	0.53
1:D:176:ILE:O	1:D:176:ILE:HG22	2.09	0.53
1:D:20:LYS:O	1:D:22:ILE:HG23	2.09	0.53
1:C:31:PHE:CE2	1:C:187:MET:HE1	2.44	0.53
1:C:296:ALA:O	1:C:297:ASP:HB2	2.08	0.53
1:C:65:LYS:O	1:C:67:MET:HG2	2.09	0.53
1:D:138:GLN:O	1:D:142:VAL:HG23	2.09	0.53
1:D:117:VAL:HG21	1:D:182:ARG:HH22	1.74	0.53
1:D:80:VAL:HG22	1:D:80:VAL:O	2.09	0.53
1:A:208:ASP:HB2	1:A:229:PHE:CE2	2.44	0.53
1:B:291:LEU:HD11	1:B:348:PRO:HG3	1.91	0.53
1:D:157:LEU:HB3	1:D:160:PRO:CG	2.39	0.53
1:D:249:THR:HG21	1:D:275:VAL:HG13	1.90	0.53
1:B:33:VAL:CG2	1:B:201:ALA:HB2	2.39	0.53
1:B:92:VAL:HB	1:B:128:ASP:O	2.09	0.53
1:D:139:ARG:CG	1:D:140:GLN:N	2.72	0.52
1:D:91:SER:N	1:D:94:GLU:HB3	2.23	0.52
1:A:240:ASN:O	1:A:284:GLY:HA2	2.10	0.52
1:A:237:PRO:HG3	1:A:315:GLN:HE22	1.73	0.52
1:B:123:LEU:CD2	1:B:141:ARG:HG2	2.36	0.52
1:B:305:GLN:HG3	1:B:326:ASN:OD1	2.08	0.52
1:C:261:PRO:O	1:C:262:ASN:CG	2.47	0.52
1:C:64:GLU:O	1:C:65:LYS:HD3	2.09	0.52
1:A:90:LEU:HB3	1:A:94:GLU:HB3	1.91	0.52
1:A:99:GLY:O	1:A:101:LYS:N	2.43	0.52
1:B:336:LEU:N	1:B:336:LEU:HD12	2.18	0.52
1:C:298:VAL:HG11	1:C:347:LEU:HB3	1.92	0.52
1:A:42:LYS:NZ	1:A:192:HIS:CE1	2.77	0.52
1:B:260:MET:HB3	1:B:261:PRO:CD	2.39	0.52
1:C:11:LYS:HB3	1:C:19:SER:HB3	1.91	0.52
1:D:271:GLU:CD	1:D:273:ARG:NH1	2.63	0.52
1:D:96:MET:SD	1:D:142:VAL:HG13	2.49	0.52
1:B:48:MET:HG2	1:B:53:GLU:HB2	1.92	0.52
1:B:97:SER:O	1:B:99:GLY:N	2.35	0.52
1:C:105:ALA:O	1:C:106:LYS:HB2	2.09	0.52
1:C:151:GLU:HG2	1:C:183:LEU:HD21	1.92	0.52
1:A:261:PRO:C	1:A:263:ARG:H	2.13	0.52
1:B:100:LEU:CD2	1:B:109:VAL:HB	2.40	0.52
1:D:38:SER:OG	1:D:39:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:PRO:O	1:D:72:PRO:O	2.28	0.52
1:A:271:GLU:HG2	1:A:273:ARG:NH1	2.25	0.52
1:A:314:THR:CG2	1:A:316:ILE:HD11	2.40	0.52
1:B:183:LEU:O	1:B:185:ARG:N	2.41	0.52
1:D:117:VAL:CG2	1:D:182:ARG:HH22	2.23	0.52
1:D:121:LEU:HD11	1:D:148:LEU:CD2	2.39	0.52
1:D:291:LEU:HD12	1:D:348:PRO:HG3	1.92	0.52
1:A:31:PHE:CE2	1:A:187:MET:HE1	2.45	0.51
1:B:189:TYR:HD2	1:B:190:VAL:N	2.09	0.51
1:C:100:LEU:HG	1:C:150:ALA:HA	1.92	0.51
1:C:262:ASN:O	1:C:263:ARG:C	2.48	0.51
1:B:157:LEU:N	1:B:157:LEU:HD12	2.26	0.51
1:B:6:LEU:CD2	1:B:22:ILE:HD11	2.40	0.51
1:D:92:VAL:HG23	1:D:128:ASP:C	2.31	0.51
1:D:176:ILE:O	1:D:176:ILE:CG2	2.59	0.51
1:A:241:PHE:HA	1:A:283:LEU:O	2.09	0.51
1:A:302:GLY:HA3	1:A:319:GLN:O	2.10	0.51
1:B:4:VAL:HG23	1:B:154:VAL:HG11	1.93	0.51
1:C:248:ALA:HB3	1:C:255:GLN:NE2	2.25	0.51
1:C:92:VAL:O	1:C:95:ASN:O	2.28	0.51
1:B:4:VAL:CG2	1:B:154:VAL:HG11	2.40	0.51
1:C:105:ALA:CB	1:C:109:VAL:HG21	2.39	0.51
1:C:95:ASN:O	1:C:96:MET:CB	2.55	0.51
1:C:31:PHE:CD2	1:C:187:MET:HE1	2.46	0.51
1:D:296:ALA:HA	1:D:299:ILE:HD11	1.92	0.51
1:A:10:THR:HA	1:A:19:SER:O	2.11	0.51
1:B:305:GLN:CG	1:B:319:GLN:HB2	2.41	0.51
1:B:76:GLY:O	1:B:153:SER:HB3	2.11	0.51
1:D:166:ALA:O	1:D:167:ALA:HB3	2.10	0.51
1:D:80:VAL:HG21	1:D:144:ILE:HG22	1.91	0.51
1:D:173:ARG:NE	1:D:196:GLU:HG3	2.13	0.51
1:D:314:THR:OG1	1:D:334:VAL:O	2.23	0.51
1:A:132:LYS:O	1:A:134:LEU:HB2	2.11	0.51
1:B:110:ILE:HA	1:B:114:VAL:CG2	2.41	0.51
1:B:89:HIS:CG	1:B:90:LEU:H	2.29	0.51
1:C:246:VAL:CG1	1:C:279:ALA:HB3	2.41	0.51
1:C:246:VAL:HG12	1:C:281:MET:HE2	1.92	0.51
1:D:183:LEU:N	1:D:183:LEU:HD23	2.26	0.51
1:B:11:LYS:HD2	1:B:12:ALA:H	1.75	0.51
1:B:347:LEU:HD13	1:B:347:LEU:O	2.11	0.51
1:D:122:GLN:HB3	1:D:141:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ASN:O	1:D:263:ARG:C	2.49	0.51
1:A:251:ILE:O	1:A:252:ASP:OD1	2.28	0.50
1:B:193:ASP:CG	1:B:196:GLU:HB2	2.31	0.50
1:C:159:GLU:N	1:C:160:PRO:HD3	2.26	0.50
1:C:252:ASP:HB2	1:C:365:LEU:HD12	1.91	0.50
1:D:246:VAL:HB	1:D:281:MET:HE2	1.92	0.50
1:D:80:VAL:HB	1:D:147:THR:HG21	1.93	0.50
1:B:161:LEU:CD2	1:B:161:LEU:H	2.07	0.50
1:B:208:ASP:HB2	1:B:229:PHE:CE2	2.46	0.50
1:C:320:ILE:HG23	1:C:321:PRO:HD2	1.93	0.50
1:A:179:LEU:HD23	1:A:179:LEU:C	2.31	0.50
1:C:96:MET:CE	1:C:142:VAL:HG13	2.42	0.50
1:B:11:LYS:HD2	1:B:12:ALA:N	2.27	0.50
1:C:296:ALA:O	1:C:297:ASP:CB	2.59	0.50
1:A:217:LYS:HG3	1:A:220:GLU:OE1	2.11	0.50
1:D:122:GLN:HB3	1:D:141:ARG:HH12	1.76	0.50
1:D:351:ARG:HA	1:D:364:ARG:NH2	2.25	0.50
1:D:68:ASN:ND2	1:D:68:ASN:N	2.54	0.50
1:A:22:ILE:CD1	1:A:45:LEU:HD21	2.40	0.50
1:A:62:ILE:HB	1:A:67:MET:HG3	1.93	0.50
1:B:82:GLN:O	1:B:144:ILE:HD11	2.12	0.50
1:C:80:VAL:CG1	1:C:157:LEU:HD22	2.41	0.50
1:D:86:LEU:HD11	1:D:139:ARG:HG3	1.94	0.50
1:A:291:LEU:HB3	1:A:292:PRO:HD2	1.94	0.50
1:B:123:LEU:CD2	1:B:126:LEU:HD12	2.42	0.50
1:B:358:ASP:HB3	1:B:360:THR:HG23	1.93	0.50
1:C:148:LEU:HD23	1:C:155:PHE:HE2	1.76	0.50
1:D:251:ILE:O	1:D:252:ASP:OD2	2.30	0.50
1:A:141:ARG:HG2	1:A:172:MET:HE2	1.94	0.50
1:B:92:VAL:HG11	1:B:126:LEU:O	2.12	0.50
1:D:271:GLU:OE1	1:D:273:ARG:NH1	2.44	0.50
1:A:254:VAL:HG23	1:A:272:SER:HB2	1.94	0.49
1:A:261:PRO:C	1:A:263:ARG:N	2.65	0.49
1:B:329:TYR:HE2	1:B:331:GLN:NE2	2.10	0.49
1:A:292:PRO:O	1:A:293:SER:HB3	2.12	0.49
1:A:95:ASN:O	1:A:96:MET:CB	2.54	0.49
1:C:67:MET:HE1	1:C:75:ARG:HA	1.91	0.49
1:D:197:ALA:O	1:D:204:ILE:HD11	2.12	0.49
1:D:227:ASP:OD1	1:D:230:VAL:HG23	2.12	0.49
1:D:238:LYS:HG2	1:D:239:MET:O	2.12	0.49
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:O	1:A:185:ARG:N	2.36	0.49
1:B:190:VAL:O	1:B:191:THR:HG23	2.13	0.49
1:C:159:GLU:HG3	1:C:162:SER:HB2	1.93	0.49
1:A:331:GLN:OE1	1:A:335:VAL:CG2	2.61	0.49
1:D:134:LEU:N	1:D:134:LEU:HD12	2.27	0.49
1:D:86:LEU:CD1	1:D:86:LEU:H	2.20	0.49
1:B:329:TYR:CE2	1:B:331:GLN:NE2	2.80	0.49
1:B:11:LYS:HG2	1:B:48:MET:SD	2.53	0.49
1:C:228:ARG:HH11	1:C:228:ARG:CG	2.26	0.49
1:B:69:ASP:O	1:B:71:PRO:HD3	2.13	0.49
1:D:147:THR:O	1:D:150:ALA:HB3	2.13	0.49
1:A:46:LEU:HD22	1:A:190:VAL:CG2	2.43	0.49
1:C:129:ARG:HG3	1:C:130:LYS:H	1.76	0.49
1:C:217:LYS:O	1:C:220:GLU:HB2	2.12	0.49
1:C:298:VAL:HG12	1:C:347:LEU:HB3	1.93	0.49
1:A:323:ILE:HG22	1:A:325:GLN:O	2.13	0.49
1:A:26:ILE:HG23	1:A:32:VAL:HG21	1.95	0.49
1:A:99:GLY:C	1:A:101:LYS:N	2.66	0.49
1:B:309:GLN:CD	1:B:314:THR:HG23	2.34	0.49
1:D:304:VAL:HG23	1:D:341:ALA:O	2.13	0.49
1:B:80:VAL:HG11	1:B:144:ILE:HG23	1.95	0.48
1:C:259:PRO:O	1:C:260:MET:O	2.31	0.48
1:B:100:LEU:HD12	1:B:149:VAL:O	2.12	0.48
1:C:183:LEU:H	1:C:183:LEU:HD12	1.78	0.48
1:A:95:ASN:C	1:A:97:SER:H	2.16	0.48
1:B:290:LEU:HD11	1:B:327:LEU:HD21	1.95	0.48
1:D:59:ASP:HA	1:D:68:ASN:OD1	2.13	0.48
1:D:6:LEU:HB3	1:D:9:VAL:HG21	1.96	0.48
1:B:121:LEU:C	1:B:123:LEU:H	2.15	0.48
1:B:270:VAL:HG12	1:B:364:ARG:HA	1.96	0.48
1:C:217:LYS:N	1:C:220:GLU:OE1	2.41	0.48
1:A:86:LEU:O	1:A:88:PRO:HD3	2.13	0.48
1:B:175:GLU:O	1:B:178:ARG:HB3	2.14	0.48
1:C:306:VAL:HB	1:C:317:HIS:HB2	1.94	0.48
1:D:144:ILE:C	1:D:148:LEU:HD13	2.34	0.48
1:D:191:THR:HB	1:D:193:ASP:H	1.78	0.48
1:B:204:ILE:HB	1:B:221:LEU:HD11	1.95	0.48
1:B:97:SER:C	1:B:99:GLY:H	2.17	0.48
1:D:87:TYR:CZ	1:D:98:PHE:CE2	3.01	0.48
1:A:227:ASP:OD1	1:A:230:VAL:HG23	2.14	0.48
1:A:327:LEU:CD2	1:A:345:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:HG	1:D:150:ALA:HA	1.96	0.48
1:D:307:VAL:HG12	1:D:309:GLN:NE2	2.27	0.48
1:D:96:MET:HE1	1:D:121:LEU:HD12	1.94	0.48
1:B:289:HIS:ND1	1:B:351:ARG:HG2	2.29	0.48
1:B:80:VAL:CG1	1:B:84:TYR:HD1	2.26	0.48
1:C:103:ALA:O	1:C:104:GLY:O	2.32	0.48
1:C:253:GLN:O	1:C:268:LEU:O	2.32	0.48
1:C:55:ILE:HD11	1:C:60:LEU:HD22	1.95	0.48
1:A:252:ASP:HB2	1:A:365:LEU:HD11	1.95	0.48
1:B:107:LYS:HB2	1:B:107:LYS:NZ	2.28	0.48
1:B:118:ALA:HA	1:B:123:LEU:HD12	1.95	0.48
1:A:311:GLY:O	1:B:222:TYR:CE2	2.67	0.48
1:C:182:ARG:HH21	1:C:183:LEU:HD11	1.78	0.48
1:C:183:LEU:N	1:C:183:LEU:HD12	2.29	0.48
1:D:63:GLY:O	1:D:64:GLU:HB2	2.13	0.48
1:A:314:THR:HG22	1:A:316:ILE:CD1	2.44	0.47
1:B:101:LYS:HB3	1:B:101:LYS:HZ2	1.79	0.47
1:B:123:LEU:HD21	1:B:141:ARG:CB	2.44	0.47
1:C:42:LYS:CE	1:C:192:HIS:NE2	2.77	0.47
1:B:254:VAL:HG21	1:B:272:SER:HA	1.95	0.47
1:B:56:THR:O	1:B:57:SER:CB	2.60	0.47
1:A:50:ALA:HB2	1:A:156:LEU:HD12	1.96	0.47
1:C:252:ASP:HA	1:C:272:SER:HB3	1.96	0.47
1:B:80:VAL:CG1	1:B:144:ILE:HG23	2.44	0.47
1:B:31:PHE:HE1	1:B:189:TYR:HB2	1.79	0.47
1:B:68:ASN:N	1:B:68:ASN:HD22	2.12	0.47
1:C:42:LYS:NZ	1:C:192:HIS:CE1	2.82	0.47
1:D:159:GLU:N	1:D:160:PRO:CD	2.76	0.47
1:C:311:GLY:O	1:D:222:TYR:CE2	2.67	0.47
1:D:271:GLU:HB3	1:D:362:CYS:HB3	1.96	0.47
1:A:86:LEU:HD11	1:A:142:VAL:HB	1.96	0.47
1:B:167:ALA:C	1:B:169:ARG:H	2.18	0.47
1:B:305:GLN:NE2	1:B:319:GLN:HB2	2.29	0.47
1:C:305:GLN:CG	1:C:319:GLN:HB2	2.45	0.47
1:C:51:GLY:O	1:C:72:PRO:HG3	2.14	0.47
1:C:93:ALA:O	1:C:97:SER:HB3	2.15	0.47
1:C:87:TYR:N	1:C:95:ASN:HD21	2.12	0.47
1:A:206:VAL:HG21	1:A:234:ILE:HD11	1.95	0.47
1:B:123:LEU:O	1:B:124:ALA:HB2	2.15	0.47
1:C:99:GLY:O	1:C:102:LEU:CB	2.57	0.47
1:D:351:ARG:HD2	1:D:368:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:CD2	1:A:172:MET:SD	3.02	0.47
1:A:46:LEU:HD22	1:A:190:VAL:HG23	1.96	0.47
1:A:208:ASP:HB2	1:A:229:PHE:CZ	2.49	0.47
1:B:65:LYS:HD3	1:B:65:LYS:N	2.30	0.47
1:C:63:GLY:O	1:C:64:GLU:CB	2.60	0.47
1:D:123:LEU:C	1:D:125:HIS:H	2.17	0.47
1:D:271:GLU:HG3	1:D:273:ARG:CB	2.45	0.47
1:D:51:GLY:C	1:D:53:GLU:H	2.18	0.47
1:A:31:PHE:CE2	1:A:187:MET:CE	2.97	0.47
1:A:34:PHE:CD2	1:A:205:VAL:HG11	2.50	0.47
1:B:110:ILE:HG23	1:B:114:VAL:HG11	1.95	0.47
1:D:211:ARG:HG3	1:D:212:VAL:N	2.27	0.47
1:A:290:LEU:HD13	1:A:345:ILE:HD12	1.97	0.47
1:A:296:ALA:O	1:A:297:ASP:HB2	2.14	0.47
1:A:88:PRO:HA	1:A:131:PRO:HG2	1.95	0.47
1:B:11:LYS:HG3	1:B:18:VAL:CG2	2.45	0.47
1:B:198:MET:HE3	1:B:218:PRO:HB3	1.97	0.47
1:A:121:LEU:O	1:A:123:LEU:HG	2.15	0.47
1:A:262:ASN:O	1:A:263:ARG:C	2.53	0.47
1:A:285:ILE:O	1:A:285:ILE:HG23	2.15	0.47
1:B:262:ASN:O	1:B:263:ARG:C	2.54	0.47
1:B:80:VAL:HG13	1:B:84:TYR:CE1	2.50	0.47
1:C:198:MET:CE	1:C:218:PRO:C	2.78	0.47
1:D:320:ILE:CD1	1:D:327:LEU:HD22	2.43	0.47
1:A:126:LEU:HD11	1:A:138:GLN:OE1	2.15	0.47
1:B:135:SER:HB2	1:B:138:GLN:HB2	1.97	0.47
1:C:260:MET:C	1:C:261:PRO:O	2.52	0.47
1:C:283:LEU:HD23	1:C:283:LEU:C	2.35	0.47
1:C:29:GLY:HA2	1:C:184:GLY:O	2.15	0.47
1:D:91:SER:OG	1:D:128:ASP:HA	2.15	0.47
1:B:179:LEU:HD21	1:B:183:LEU:HD12	1.97	0.46
1:C:117:VAL:O	1:C:121:LEU:HG	2.16	0.46
1:D:239:MET:CE	1:D:286:ARG:HG3	2.45	0.46
1:B:270:VAL:O	1:B:272:SER:N	2.48	0.46
1:C:157:LEU:HB3	1:C:160:PRO:CG	2.46	0.46
1:D:161:LEU:HD13	1:D:172:MET:HB2	1.97	0.46
1:D:306:VAL:HB	1:D:317:HIS:CG	2.50	0.46
1:A:97:SER:O	1:A:99:GLY:O	2.33	0.46
1:B:170:VAL:O	1:B:174:ILE:HG13	2.15	0.46
1:B:144:ILE:C	1:B:146:ARG:H	2.19	0.46
1:B:146:ARG:HG3	1:B:146:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:HG12	1:B:18:VAL:N	2.31	0.46
1:D:208:ASP:HB2	1:D:229:PHE:CE2	2.49	0.46
1:B:45:LEU:HA	1:B:48:MET:HE2	1.94	0.46
1:A:165:ASP:O	1:A:165:ASP:OD2	2.34	0.46
1:A:271:GLU:O	1:A:272:SER:HB3	2.15	0.46
1:A:62:ILE:C	1:A:64:GLU:N	2.69	0.46
1:A:61:PHE:HD2	1:A:64:GLU:O	1.99	0.46
1:B:90:LEU:HB3	1:B:94:GLU:HB2	1.98	0.46
1:C:149:VAL:HG23	1:C:149:VAL:O	2.15	0.46
1:B:121:LEU:HA	1:B:168:LEU:HD22	1.97	0.46
1:B:272:SER:O	1:B:273:ARG:O	2.33	0.46
1:C:272:SER:O	1:C:273:ARG:O	2.33	0.46
1:C:329:TYR:CE2	1:C:331:GLN:HB2	2.51	0.46
1:D:249:THR:HG22	1:D:254:VAL:HG22	1.97	0.46
1:D:335:VAL:HG12	1:D:337:VAL:HG23	1.98	0.46
1:D:95:ASN:O	1:D:97:SER:N	2.42	0.46
1:B:118:ALA:HB1	1:B:123:LEU:CB	2.40	0.46
1:C:120:VAL:HB	1:C:175:GLU:CD	2.36	0.46
1:C:261:PRO:C	1:C:263:ARG:N	2.67	0.46
1:A:34:PHE:CE2	1:A:205:VAL:HG11	2.51	0.46
1:B:165:ASP:C	1:B:167:ALA:N	2.70	0.46
1:B:171:GLN:HA	1:B:174:ILE:HD12	1.97	0.46
1:B:178:ARG:HA	1:B:181:LYS:HE3	1.97	0.46
1:D:110:ILE:HA	1:D:114:VAL:HB	1.98	0.46
1:D:350:GLU:CD	1:D:350:GLU:H	2.14	0.46
1:D:80:VAL:HG13	1:D:80:VAL:O	2.16	0.46
1:B:109:VAL:HG23	1:B:110:ILE:N	2.32	0.46
1:B:45:LEU:C	1:B:45:LEU:HD23	2.36	0.46
1:B:5:GLN:C	1:B:6:LEU:HD12	2.36	0.46
1:C:327:LEU:HD23	1:C:345:ILE:CD1	2.42	0.46
1:B:289:HIS:ND1	1:B:351:ARG:CG	2.79	0.45
1:B:261:PRO:C	1:B:263:ARG:N	2.67	0.45
1:B:283:LEU:C	1:B:283:LEU:HD23	2.37	0.45
1:C:42:LYS:HZ1	1:C:192:HIS:CE1	2.34	0.45
1:D:114:VAL:CG2	1:D:149:VAL:HG11	2.40	0.45
1:D:228:ARG:CG	1:D:228:ARG:HH11	2.29	0.45
1:A:237:PRO:O	1:A:287:PRO:CG	2.65	0.45
1:D:121:LEU:HD21	1:D:148:LEU:HD21	1.97	0.45
1:B:131:PRO:O	1:B:134:LEU:HG	2.16	0.45
1:B:271:GLU:HG3	1:B:273:ARG:HB2	1.98	0.45
1:B:320:ILE:CG2	1:B:323:ILE:HD12	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:CA	1:B:48:MET:CE	2.88	0.45
1:C:198:MET:SD	1:C:218:PRO:HB3	2.56	0.45
1:A:175:GLU:OE1	1:A:178:ARG:NH2	2.49	0.45
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.82	0.45
1:B:110:ILE:HA	1:B:114:VAL:CB	2.47	0.45
1:B:86:LEU:HG	1:B:142:VAL:O	2.17	0.45
1:B:80:VAL:CG1	1:B:144:ILE:O	2.63	0.45
1:B:261:PRO:C	1:B:263:ARG:H	2.19	0.45
1:C:182:ARG:HB3	1:C:183:LEU:HD12	1.97	0.45
1:D:166:ALA:C	1:D:168:LEU:H	2.20	0.45
1:A:20:LYS:O	1:A:21:ASP:C	2.55	0.45
1:A:39:GLY:C	1:A:41:GLY:N	2.70	0.45
1:B:179:LEU:CG	1:B:183:LEU:HD12	2.46	0.45
1:B:293:SER:C	1:B:295:ILE:N	2.68	0.45
1:C:285:ILE:HG23	1:C:285:ILE:O	2.16	0.45
1:C:289:HIS:O	1:C:348:PRO:HG2	2.17	0.45
1:C:96:MET:HG2	1:C:96:MET:O	2.16	0.45
1:A:96:MET:HA	1:A:146:ARG:CA	2.47	0.45
1:B:165:ASP:OD2	1:B:167:ALA:HB3	2.17	0.45
1:B:6:LEU:HD23	1:B:22:ILE:HD11	1.99	0.45
1:C:297:ASP:C	1:C:298:VAL:HG23	2.36	0.45
1:D:70:THR:O	1:D:75:ARG:NH1	2.50	0.45
1:A:211:ARG:HG3	1:A:212:VAL:N	2.31	0.45
1:A:65:LYS:HD3	1:A:65:LYS:H	1.78	0.45
1:B:189:TYR:CE2	1:B:191:THR:HG23	2.48	0.45
1:D:185:ARG:O	1:D:187:MET:HG3	2.16	0.45
1:D:285:ILE:O	1:D:285:ILE:HG23	2.17	0.45
1:C:331:GLN:OE1	1:C:335:VAL:HG21	2.16	0.44
1:D:300:LEU:N	1:D:300:LEU:HD12	2.32	0.44
1:A:191:THR:HB	1:A:193:ASP:H	1.82	0.44
1:A:293:SER:C	1:A:295:ILE:N	2.71	0.44
1:B:96:MET:CA	1:B:146:ARG:HA	2.13	0.44
1:B:20:LYS:HE2	1:B:211:ARG:NH2	2.33	0.44
1:B:183:LEU:C	1:B:185:ARG:N	2.68	0.44
1:B:227:ASP:HB2	1:B:359:GLY:O	2.18	0.44
1:C:29:GLY:O	1:C:180:HIS:HE1	2.00	0.44
1:B:355:PHE:CD1	1:B:355:PHE:N	2.85	0.44
1:B:88:PRO:HA	1:B:132:LYS:HB2	1.98	0.44
1:C:185:ARG:HG2	1:C:185:ARG:HH11	1.82	0.44
1:D:6:LEU:HB3	1:D:9:VAL:CG2	2.47	0.44
1:B:89:HIS:CD2	1:B:90:LEU:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:LEU:HD23	1:D:283:LEU:C	2.38	0.44
1:D:42:LYS:CE	1:D:192:HIS:NE2	2.80	0.44
1:D:43:SER:O	1:D:44:THR:C	2.55	0.44
1:D:96:MET:HE2	1:D:121:LEU:HD12	1.99	0.44
1:A:110:ILE:O	1:A:112:GLN:N	2.50	0.44
1:A:96:MET:O	1:A:149:VAL:HG21	2.18	0.44
1:B:77:VAL:HG23	1:B:78:GLY:N	2.33	0.44
1:C:208:ASP:HB2	1:C:229:PHE:CE2	2.52	0.44
1:C:260:MET:O	1:C:261:PRO:O	2.36	0.44
1:A:11:LYS:HE3	1:A:13:TRP:CZ2	2.53	0.44
1:B:157:LEU:HD11	1:B:187:MET:HE3	1.99	0.44
1:B:42:LYS:NZ	1:B:192:HIS:NE2	2.62	0.44
1:C:271:GLU:HB2	1:C:363:ARG:HB3	1.99	0.44
1:C:45:LEU:CD2	1:C:48:MET:CE	2.88	0.44
1:D:159:GLU:HG3	1:D:162:SER:HB2	2.00	0.44
1:D:255:GLN:HA	1:D:266:VAL:O	2.18	0.44
1:D:86:LEU:HD12	1:D:86:LEU:N	2.25	0.44
1:A:90:LEU:HG	1:A:94:GLU:CB	2.48	0.44
1:B:80:VAL:HG21	1:B:148:LEU:HD12	1.99	0.44
1:C:15:GLU:OE1	1:C:15:GLU:HA	2.17	0.44
1:B:110:ILE:O	1:B:115:ASN:OD1	2.36	0.44
1:B:132:LYS:HA	1:B:139:ARG:HH11	1.81	0.44
1:B:228:ARG:CG	1:B:228:ARG:HH11	2.23	0.44
1:B:238:LYS:HG2	1:B:239:MET:N	2.32	0.44
1:B:57:SER:OG	1:B:58:GLY:N	2.51	0.44
1:A:222:TYR:OH	1:A:288:GLU:OE1	2.29	0.43
1:B:253:GLN:CB	1:B:267:TRP:CE3	3.00	0.43
1:B:304:VAL:HG12	1:B:339:GLU:HA	2.00	0.43
1:B:55:ILE:HG22	1:B:57:SER:O	2.18	0.43
1:B:87:TYR:CE2	1:B:98:PHE:CE1	3.06	0.43
1:D:77:VAL:O	1:D:152:PRO:HG3	2.17	0.43
1:D:293:SER:HB2	1:D:344:ALA:O	2.18	0.43
1:A:253:GLN:HB3	1:A:267:TRP:CZ3	2.53	0.43
1:B:72:PRO:O	1:B:73:ALA:C	2.56	0.43
1:B:95:ASN:CB	1:B:142:VAL:HG13	2.49	0.43
1:C:134:LEU:HB2	1:C:139:ARG:HG3	1.99	0.43
1:D:42:LYS:NZ	1:D:192:HIS:NE2	2.63	0.43
1:D:65:LYS:HD3	1:D:65:LYS:N	2.33	0.43
1:A:107:LYS:O	1:A:111:ASN:HB3	2.17	0.43
1:B:271:GLU:HG3	1:B:273:ARG:H	1.83	0.43
1:C:20:LYS:N	1:C:20:LYS:HD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:VAL:HG13	1:D:278:GLY:H	1.83	0.43
1:D:26:ILE:HG23	1:D:32:VAL:HG21	2.01	0.43
1:A:121:LEU:HD22	1:A:172:MET:SD	2.58	0.43
1:B:240:ASN:HD21	1:B:328:VAL:H	1.65	0.43
1:C:170:VAL:O	1:C:173:ARG:HB3	2.18	0.43
1:D:96:MET:HE1	1:D:121:LEU:CD1	2.48	0.43
1:A:65:LYS:CD	1:A:65:LYS:N	2.80	0.43
1:B:240:ASN:O	1:B:284:GLY:HA2	2.19	0.43
1:C:219:LEU:HA	1:C:219:LEU:HD12	1.87	0.43
1:D:155:PHE:CE1	1:D:179:LEU:HD21	2.53	0.43
1:A:148:LEU:HG	1:A:179:LEU:HD13	1.97	0.43
1:A:321:PRO:O	1:A:322:SER:CB	2.67	0.43
1:B:179:LEU:HD23	1:B:179:LEU:C	2.38	0.43
1:B:254:VAL:CG2	1:B:272:SER:HA	2.49	0.43
1:C:70:THR:O	1:C:75:ARG:NH1	2.52	0.43
1:A:327:LEU:HD22	1:A:345:ILE:HD11	2.01	0.43
1:A:79:MET:HG2	1:A:80:VAL:N	2.34	0.43
1:A:90:LEU:CG	1:A:94:GLU:HG2	2.24	0.43
1:B:9:VAL:HB	1:B:22:ILE:HG12	1.99	0.43
1:C:31:PHE:CE2	1:C:187:MET:CE	3.02	0.43
1:D:355:PHE:CD1	1:D:355:PHE:N	2.87	0.43
1:D:34:PHE:CE1	1:D:45:LEU:HD22	2.49	0.43
1:C:241:PHE:O	1:C:242:LEU:HD23	2.19	0.43
1:A:159:GLU:CD	1:A:191:THR:HG22	2.39	0.43
1:B:118:ALA:HA	1:B:123:LEU:CD1	2.49	0.43
1:B:242:LEU:HD21	1:B:327:LEU:HD12	2.00	0.43
1:C:158:ASP:O	1:C:159:GLU:C	2.56	0.43
1:D:268:LEU:HA	1:D:269:PRO:HD3	1.84	0.43
1:B:135:SER:C	1:B:137:GLY:H	2.22	0.42
1:B:24:LEU:N	1:B:24:LEU:HD12	2.34	0.42
1:C:174:ILE:O	1:C:175:GLU:C	2.57	0.42
1:C:271:GLU:HG2	1:C:273:ARG:NH1	2.33	0.42
1:C:246:VAL:HG11	1:C:279:ALA:HB3	2.01	0.42
1:D:238:LYS:HG2	1:D:239:MET:N	2.34	0.42
1:D:5:GLN:OE1	1:D:7:GLN:NE2	2.53	0.42
1:D:96:MET:CE	1:D:121:LEU:CD1	2.97	0.42
1:D:87:TYR:CE2	1:D:98:PHE:CE2	3.06	0.42
1:A:47:ARG:HB3	1:A:53:GLU:HG2	2.00	0.42
1:C:18:VAL:O	1:C:19:SER:HB2	2.19	0.42
1:D:123:LEU:HD11	1:D:142:VAL:HG22	1.99	0.42
1:A:260:MET:C	1:A:261:PRO:O	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASN:HA	1:B:146:ARG:HH12	1.83	0.42
1:C:234:ILE:N	1:C:234:ILE:HD12	2.34	0.42
1:C:237:PRO:HG2	1:C:330:ARG:HD2	2.01	0.42
1:C:298:VAL:HG12	1:C:347:LEU:CB	2.49	0.42
1:A:135:SER:OG	1:A:138:GLN:HG3	2.20	0.42
1:A:205:VAL:HG13	1:A:205:VAL:O	2.20	0.42
1:C:6:LEU:CD2	1:C:22:ILE:HD11	2.48	0.42
1:C:272:SER:O	1:C:272:SER:OG	2.37	0.42
1:D:51:GLY:C	1:D:53:GLU:N	2.73	0.42
1:C:105:ALA:O	1:C:109:VAL:CG1	2.67	0.42
1:C:170:VAL:O	1:C:174:ILE:HG13	2.20	0.42
1:C:33:VAL:HB	1:C:204:ILE:HG12	2.00	0.42
1:D:80:VAL:CG2	1:D:144:ILE:HA	2.43	0.42
1:D:20:LYS:O	1:D:22:ILE:N	2.53	0.42
1:D:91:SER:O	1:D:94:GLU:HB3	2.19	0.42
1:A:173:ARG:NE	1:A:196:GLU:HG3	2.28	0.42
1:A:322:SER:O	1:A:323:ILE:HG13	2.20	0.42
1:A:56:THR:O	1:A:57:SER:HB2	2.20	0.42
1:B:24:LEU:H	1:B:24:LEU:HD12	1.83	0.42
1:D:9:VAL:HB	1:D:22:ILE:HG12	2.02	0.42
1:A:96:MET:O	1:A:149:VAL:CG2	2.66	0.42
1:B:88:PRO:CB	1:B:132:LYS:HD3	2.40	0.42
1:B:46:LEU:CD2	1:B:158:ASP:HB2	2.49	0.42
1:B:51:GLY:C	1:B:53:GLU:H	2.23	0.42
1:B:9:VAL:HG13	1:B:55:ILE:HG23	2.01	0.42
1:C:211:ARG:HG3	1:C:212:VAL:H	1.85	0.42
1:C:300:LEU:N	1:C:300:LEU:CD1	2.81	0.42
1:D:117:VAL:HG22	1:D:182:ARG:NH1	2.29	0.42
1:B:228:ARG:NH1	1:B:228:ARG:CG	2.81	0.42
1:B:323:ILE:O	1:B:324:ARG:C	2.57	0.42
1:B:347:LEU:HD21	1:B:352:CYS:SG	2.60	0.42
1:B:43:SER:O	1:B:46:LEU:HB3	2.19	0.42
1:B:88:PRO:O	1:B:132:LYS:HB2	2.20	0.42
1:B:97:SER:C	1:B:99:GLY:N	2.72	0.42
1:C:50:ALA:HB2	1:C:156:LEU:CD1	2.50	0.42
1:C:253:GLN:O	1:C:254:VAL:CB	2.67	0.42
1:D:110:ILE:N	1:D:110:ILE:CD1	2.82	0.42
1:A:272:SER:O	1:A:275:VAL:HG12	2.20	0.42
1:A:291:LEU:HB2	1:A:346:GLY:HA3	2.02	0.42
1:A:96:MET:HA	1:A:146:ARG:HA	2.02	0.42
1:D:6:LEU:N	1:D:6:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:CG2	1:A:206:VAL:HG22	2.50	0.41
1:C:161:LEU:HB3	1:C:169:ARG:HD2	2.02	0.41
1:D:86:LEU:HD11	1:D:139:ARG:CG	2.49	0.41
1:D:228:ARG:NH1	1:D:228:ARG:HG2	2.33	0.41
1:B:86:LEU:HA	1:B:146:ARG:HH21	1.84	0.41
1:D:273:ARG:HG2	1:D:274:ASP:N	2.36	0.41
1:D:295:ILE:CD1	1:D:295:ILE:N	2.82	0.41
1:B:48:MET:HG2	1:B:53:GLU:CB	2.50	0.41
1:C:13:TRP:O	1:C:16:VAL:HG22	2.20	0.41
1:D:159:GLU:H	1:D:160:PRO:HD3	1.81	0.41
1:D:213:ALA:HB1	1:D:230:VAL:HG22	2.01	0.41
1:D:246:VAL:HG13	1:D:278:GLY:N	2.34	0.41
1:A:102:LEU:O	1:A:103:ALA:HB3	2.20	0.41
1:A:237:PRO:O	1:A:238:LYS:O	2.38	0.41
1:B:289:HIS:CG	1:B:351:ARG:HG2	2.55	0.41
1:B:323:ILE:HG21	1:B:323:ILE:HD13	1.86	0.41
1:B:33:VAL:HA	1:B:189:TYR:O	2.21	0.41
1:B:87:TYR:HE2	1:B:98:PHE:CE1	2.37	0.41
1:C:44:THR:O	1:C:47:ARG:HB2	2.20	0.41
1:D:347:LEU:CD2	1:D:352:CYS:SG	3.07	0.41
1:D:56:THR:O	1:D:57:SER:HB2	2.20	0.41
1:D:67:MET:O	1:D:69:ASP:N	2.53	0.41
1:D:72:PRO:HB2	1:D:73:ALA:H	1.52	0.41
1:B:89:HIS:CG	1:B:90:LEU:N	2.89	0.41
1:D:321:PRO:O	1:D:322:SER:OG	2.31	0.41
1:A:197:ALA:HB1	1:A:204:ILE:HD11	2.02	0.41
1:B:40:CYS:HA	1:B:209:ALA:H	1.86	0.41
1:C:171:GLN:O	1:C:174:ILE:HB	2.21	0.41
1:D:52:LEU:HD12	1:D:81:PHE:HE2	1.85	0.41
1:B:141:ARG:HH11	1:B:141:ARG:HG2	1.85	0.41
1:B:306:VAL:H	1:B:317:HIS:HB2	1.86	0.41
1:D:139:ARG:HG3	1:D:139:ARG:HH11	1.86	0.41
1:D:8:ASN:O	1:D:58:GLY:HA3	2.20	0.41
1:A:134:LEU:O	1:A:139:ARG:NH1	2.54	0.41
1:A:272:SER:OG	1:A:272:SER:O	2.39	0.41
1:B:117:VAL:C	1:B:119:GLU:N	2.74	0.41
1:B:189:TYR:CD2	1:B:190:VAL:N	2.87	0.41
1:B:285:ILE:HG12	1:B:347:LEU:HD23	2.02	0.41
1:B:61:PHE:N	1:B:61:PHE:CD1	2.89	0.41
1:C:281:MET:SD	1:C:354:LEU:HD21	2.58	0.41
1:D:114:VAL:O	1:D:114:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ILE:HG13	1:D:22:ILE:O	2.20	0.41
1:A:98:PHE:HD1	1:A:101:LYS:HZ1	1.66	0.41
1:A:337:VAL:HG21	1:A:343:PHE:CE1	2.56	0.41
1:A:40:CYS:SG	1:A:42:LYS:HG2	2.61	0.41
1:B:34:PHE:CE1	1:B:45:LEU:HD22	2.42	0.41
1:C:71:PRO:HA	1:C:72:PRO:HD3	1.89	0.41
1:A:308:GLU:OE2	1:B:199:THR:HG21	2.21	0.41
1:A:44:THR:O	1:A:48:MET:HG3	2.20	0.41
1:B:191:THR:HB	1:B:193:ASP:H	1.86	0.41
1:B:334:VAL:O	1:B:335:VAL:HB	2.21	0.41
1:C:31:PHE:HD2	1:C:187:MET:CE	2.27	0.41
1:C:350:GLU:CD	1:C:350:GLU:H	2.24	0.41
1:C:5:GLN:C	1:C:6:LEU:HD12	2.41	0.41
1:D:49:ILE:HG22	1:D:49:ILE:O	2.21	0.41
1:B:109:VAL:O	1:B:114:VAL:HG23	2.19	0.40
1:B:193:ASP:OD1	1:B:196:GLU:HB2	2.21	0.40
1:B:342:THR:O	1:B:342:THR:HG23	2.21	0.40
1:C:291:LEU:HB3	1:C:292:PRO:HD2	2.03	0.40
1:D:84:TYR:CB	1:D:146:ARG:HH22	2.31	0.40
1:D:173:ARG:NH2	1:D:196:GLU:OE2	2.54	0.40
1:D:249:THR:O	1:D:250:ALA:HB2	2.21	0.40
1:D:271:GLU:HG3	1:D:273:ARG:HB2	2.02	0.40
1:D:31:PHE:HE1	1:D:189:TYR:HB2	1.85	0.40
1:D:51:GLY:O	1:D:53:GLU:N	2.53	0.40
1:A:65:LYS:O	1:A:67:MET:HG2	2.21	0.40
1:B:179:LEU:HG	1:B:183:LEU:HD12	2.03	0.40
1:C:112:GLN:HG3	1:C:113:ARG:N	2.37	0.40
1:C:217:LYS:HB2	1:C:220:GLU:OE1	2.21	0.40
1:A:159:GLU:OE2	1:A:191:THR:HG22	2.21	0.40
1:A:263:ARG:NH1	1:A:263:ARG:HG2	2.35	0.40
1:A:281:MET:HE3	1:A:354:LEU:HD21	2.02	0.40
1:B:314:THR:CG2	1:B:334:VAL:O	2.69	0.40
1:B:4:VAL:HG12	1:B:5:GLN:N	2.36	0.40
1:C:157:LEU:HB3	1:C:160:PRO:HG3	2.03	0.40
1:D:139:ARG:HD3	1:D:140:GLN:N	2.36	0.40
1:D:258:LEU:HD13	1:D:260:MET:HE1	2.02	0.40
1:D:304:VAL:HG13	1:D:316:ILE:CG2	2.51	0.40
1:B:159:GLU:N	1:B:160:PRO:CD	2.81	0.40
1:C:109:VAL:CG2	1:C:110:ILE:N	2.83	0.40
1:C:259:PRO:O	1:C:260:MET:C	2.58	0.40
1:C:32:VAL:HG12	1:C:33:VAL:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:VAL:CG2	1:D:201:ALA:HB2	2.47	0.40
1:D:260:MET:HE1	1:D:300:LEU:HG	2.03	0.40
1:A:283:LEU:C	1:A:283:LEU:HD23	2.41	0.40
1:A:297:ASP:O	1:A:298:VAL:CB	2.68	0.40
1:B:252:ASP:C	1:B:253:GLN:HG2	2.41	0.40
1:B:271:GLU:HG2	1:B:273:ARG:NH1	2.36	0.40
1:C:50:ALA:HB2	1:C:156:LEU:HD12	2.02	0.40
1:D:133:ALA:O	1:D:134:LEU:HB2	2.22	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	365/381 (96%)	291 (80%)	43 (12%)	31 (8%)	1	1
1	B	365/381 (96%)	253 (69%)	63 (17%)	49 (13%)	0	0
1	C	365/381 (96%)	302 (83%)	39 (11%)	24 (7%)	1	3
1	D	365/381 (96%)	278 (76%)	55 (15%)	32 (9%)	1	1
All	All	1460/1524 (96%)	1124 (77%)	200 (14%)	136 (9%)	0	1

All (136) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	82	GLN
1	A	103	ALA
1	A	167	ALA
1	A	238	LYS
1	A	262	ASN
1	A	273	ARG

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Mol	Chain	Res	Type
1	A	296	ALA
1	A	322	SER
1	A	323	ILE
1	B	8	ASN
1	B	12	ALA
1	B	38	SER
1	B	52	LEU
1	B	57	SER
1	B	72	PRO
1	B	81	PHE
1	B	106	LYS
1	B	124	ALA
1	B	160	PRO
1	B	161	LEU
1	B	165	ASP
1	B	252	ASP
1	B	263	ARG
1	B	271	GLU
1	B	273	ARG
1	B	293	SER
1	C	19	SER
1	C	21	ASP
1	C	64	GLU
1	C	82	GLN
1	C	104	GLY
1	C	107	LYS
1	C	263	ARG
1	C	273	ARG
1	C	296	ALA
1	D	38	SER
1	D	72	PRO
1	D	73	ALA
1	D	79	MET
1	D	81	PHE
1	D	83	SER
1	D	98	PHE
1	D	102	LEU
1	D	152	PRO
1	D	184	GLY
1	D	253	GLN
1	D	263	ARG
1	D	273	ARG

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Mol	Chain	Res	Type
1	A	64	GLU
1	A	112	GLN
1	A	132	LYS
1	A	133	ALA
1	A	168	LEU
1	A	271	GLU
1	A	293	SER
1	B	21	ASP
1	B	58	GLY
1	B	73	ALA
1	B	82	GLN
1	B	86	LEU
1	B	97	SER
1	B	116	GLN
1	B	166	ALA
1	B	254	VAL
1	B	260	MET
1	B	262	ASN
1	B	333	ASP
1	C	101	LYS
1	C	103	ALA
1	C	124	ALA
1	C	271	GLU
1	C	298	VAL
1	D	21	ASP
1	D	64	GLU
1	D	68	ASN
1	D	75	ARG
1	D	97	SER
1	D	271	GLU
1	A	21	ASP
1	A	106	LYS
1	A	114	VAL
1	B	15	GLU
1	B	64	GLU
1	B	132	LYS
1	B	145	GLY
1	B	168	LEU
1	C	38	SER
1	C	111	ASN
1	C	254	VAL
1	C	297	ASP

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Mol	Chain	Res	Type
1	D	124	ALA
1	D	129	ARG
1	A	263	ARG
1	A	363	ARG
1	B	14	GLY
1	B	56	THR
1	B	79	MET
1	B	137	GLY
1	B	150	ALA
1	B	324	ARG
1	C	175	GLU
1	C	261	PRO
1	C	333	ASP
1	D	52	LEU
1	D	106	LYS
1	D	250	ALA
1	D	363	ARG
1	A	237	PRO
1	A	254	VAL
1	A	261	PRO
1	A	298	VAL
1	B	71	PRO
1	B	298	VAL
1	B	323	ILE
1	B	335	VAL
1	C	260	MET
1	D	58	GLY
1	D	274	ASP
1	D	335	VAL
1	A	102	LEU
1	A	184	GLY
1	B	104	GLY
1	D	86	LEU
1	A	236	SER
1	B	120	VAL
1	C	174	ILE
1	D	131	PRO
1	A	110	ILE
1	B	37	PRO
1	C	218	PRO
1	D	218	PRO
1	B	152	PRO

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Mol	Chain	Res	Type
1	A	218	PRO
1	B	334	VAL
1	D	114	VAL

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	312/324 (96%)	292 (94%)	20 (6%)	17	45
1	B	312/324 (96%)	289 (93%)	23 (7%)	13	37
1	C	312/324 (96%)	289 (93%)	23 (7%)	13	37
1	D	312/324 (96%)	284 (91%)	28 (9%)	9	28
All	All	1248/1296 (96%)	1154 (92%)	94 (8%)	13	37

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	65	LYS
1	A	72	PRO
1	A	94	GLU
1	A	112	GLN
1	A	115	ASN
1	A	116	GLN
1	A	178	ARG
1	A	185	ARG
1	A	236	SER
1	A	253	GLN
1	A	272	SER
1	A	288	GLU
1	A	300	LEU
1	A	327	LEU
1	A	336	LEU
1	A	347	LEU
1	A	350	GLU

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Mol	Chain	Res	Type
1	A	351	ARG
1	A	357	GLU
1	B	31	PHE
1	B	43	SER
1	B	54	THR
1	B	81	PHE
1	B	84	TYR
1	B	100	LEU
1	B	116	GLN
1	B	127	LEU
1	B	147	THR
1	B	161	LEU
1	B	171	GLN
1	B	189	TYR
1	B	191	THR
1	B	205	VAL
1	B	219	LEU
1	B	272	SER
1	B	275	VAL
1	B	294	ASP
1	B	314	THR
1	B	327	LEU
1	B	333	ASP
1	B	336	LEU
1	B	351	ARG
1	C	20	LYS
1	C	31	PHE
1	C	45	LEU
1	C	65	LYS
1	C	79	MET
1	C	86	LEU
1	C	94	GLU
1	C	100	LEU
1	C	112	GLN
1	C	126	LEU
1	C	147	THR
1	C	149	VAL
1	C	161	LEU
1	C	179	LEU
1	C	181	LYS
1	C	205	VAL
1	C	219	LEU

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Mol	Chain	Res	Type
1	C	246	VAL
1	C	333	ASP
1	C	336	LEU
1	C	347	LEU
1	C	350	GLU
1	C	351	ARG
1	D	15	GLU
1	D	31	PHE
1	D	43	SER
1	D	64	GLU
1	D	68	ASN
1	D	95	ASN
1	D	98	PHE
1	D	102	LEU
1	D	115	ASN
1	D	119	GLU
1	D	129	ARG
1	D	139	ARG
1	D	140	GLN
1	D	141	ARG
1	D	183	LEU
1	D	205	VAL
1	D	214	GLN
1	D	219	LEU
1	D	252	ASP
1	D	282	SER
1	D	287	PRO
1	D	322	SER
1	D	333	ASP
1	D	336	LEU
1	D	342	THR
1	D	347	LEU
1	D	350	GLU
1	D	351	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	111	ASN
1	A	112	GLN
1	A	240	ASN

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	264	GLN
1	A	315	GLN
1	B	5	GLN
1	B	7	GLN
1	B	68	ASN
1	B	82	GLN
1	B	115	ASN
1	B	140	GLN
1	B	240	ASN
1	B	255	GLN
1	B	262	ASN
1	B	309	GLN
1	B	317	HIS
1	B	331	GLN
1	C	5	GLN
1	C	68	ASN
1	C	95	ASN
1	C	112	GLN
1	C	138	GLN
1	C	140	GLN
1	C	240	ASN
1	C	255	GLN
1	C	264	GLN
1	C	317	HIS
1	C	331	GLN
1	C	353	HIS
1	D	23	ASN
1	D	68	ASN
1	D	116	GLN
1	D	138	GLN
1	D	163	ASN
1	D	240	ASN
1	D	255	GLN
1	D	309	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/381 (96%)	-0.29	1 (0%) 94 93	27, 53, 78, 94	0
1	B	367/381 (96%)	0.76	68 (18%) 1 1	27, 72, 139, 145	0
1	C	367/381 (96%)	-0.27	1 (0%) 94 93	29, 53, 82, 95	0
1	D	367/381 (96%)	0.15	25 (6%) 17 10	35, 68, 123, 136	0
All	All	1468/1524 (96%)	0.09	95 (6%) 18 11	27, 58, 129, 145	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	LEU	11.3
1	B	85	ALA	11.0
1	B	82	GLN	8.2
1	B	84	TYR	7.6
1	B	142	VAL	7.3
1	B	105	ALA	6.8
1	B	83	SER	6.4
1	B	95	ASN	6.3
1	B	87	TYR	6.0
1	B	113	ARG	5.6
1	B	92	VAL	5.5
1	D	106	LYS	5.4
1	B	117	VAL	5.2
1	B	122	GLN	5.1
1	D	99	GLY	5.1
1	B	139	ARG	5.0
1	B	121	LEU	4.9
1	B	127	LEU	4.9
1	B	91	SER	4.7
1	B	137	GLY	4.7
1	B	88	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	125	HIS	4.5
1	B	135	SER	4.4
1	B	128	ASP	4.3
1	B	103	ALA	4.3
1	D	100	LEU	4.3
1	D	134	LEU	4.2
1	B	141	ARG	4.1
1	B	134	LEU	4.1
1	B	107	LYS	4.1
1	D	124	ALA	4.0
1	B	101	LYS	4.0
1	B	118	ALA	3.9
1	B	138	GLN	3.9
1	B	93	ALA	3.9
1	B	14	GLY	3.8
1	B	13	TRP	3.7
1	B	86	LEU	3.7
1	B	120	VAL	3.6
1	B	133	ALA	3.4
1	B	126	LEU	3.4
1	B	8	ASN	3.4
1	B	163	ASN	3.4
1	B	296	ALA	3.4
1	D	107	LYS	3.4
1	B	94	GLU	3.3
1	D	84	TYR	3.3
1	B	114	VAL	3.3
1	B	108	GLU	3.3
1	D	324	ARG	3.3
1	D	103	ALA	3.3
1	B	129	ARG	3.2
1	B	111	ASN	3.2
1	A	296	ALA	3.1
1	B	97	SER	3.1
1	B	81	PHE	3.1
1	C	294	ASP	3.1
1	B	144	ILE	3.1
1	D	16	VAL	3.1
1	B	123	LEU	3.0
1	B	99	GLY	3.0
1	B	102	LEU	3.0
1	D	296	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	119	GLU	2.9
1	D	127	LEU	2.9
1	B	98	PHE	2.8
1	B	178	ARG	2.8
1	B	168	LEU	2.7
1	D	105	ALA	2.7
1	B	140	GLN	2.6
1	B	143	ALA	2.6
1	D	133	ALA	2.5
1	B	119	GLU	2.5
1	D	15	GLU	2.5
1	B	115	ASN	2.5
1	D	295	ILE	2.5
1	D	111	ASN	2.4
1	D	136	GLY	2.4
1	B	112	GLN	2.3
1	B	131	PRO	2.3
1	D	82	GLN	2.3
1	D	109	VAL	2.3
1	B	151	GLU	2.3
1	D	98	PHE	2.2
1	B	147	THR	2.2
1	B	89	HIS	2.2
1	D	110	ILE	2.2
1	B	124	ALA	2.2
1	B	136	GLY	2.1
1	B	106	LYS	2.1
1	B	19	SER	2.1
1	B	165	ASP	2.0
1	D	27	HIS	2.0
1	D	83	SER	2.0
1	B	90	LEU	2.0

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.