



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:34 pm GMT

PDB ID : 4L5I  
Title : Crystal structures of the LsrR proteins complexed with phospho-AI-2 and its two different analogs reveal distinct mechanisms for ligand recognition  
Authors : Ryu, K.S.; Ha, J.H.; Eo, Y.  
Deposited on : 2013-06-11  
Resolution : 3.21 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

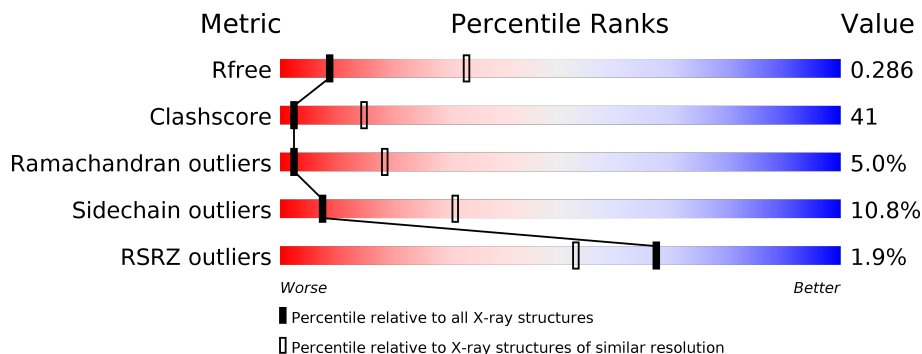
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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))
$R_{free}$	100719	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	<div> <div>3%</div> <div>36% 49% 11% .</div> </div>
1	B	318	<div> <div>43% 47% 5% . .</div> </div>
1	C	318	<div> <div>2%</div> <div>40% 51% 6% .</div> </div>
1	D	318	<div> <div>2%</div> <div>40% 47% 9% .</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9189 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 Transcriptional regulator LsrR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2286	1430	411	433	12			
1	B	308	Total	C	N	O	S	0	0	0
			2304	1440	414	438	12			
1	C	308	Total	C	N	O	S	0	0	0
			2304	1440	414	438	12			
1	D	307	Total	C	N	O	S	0	0	0
			2295	1435	413	435	12			

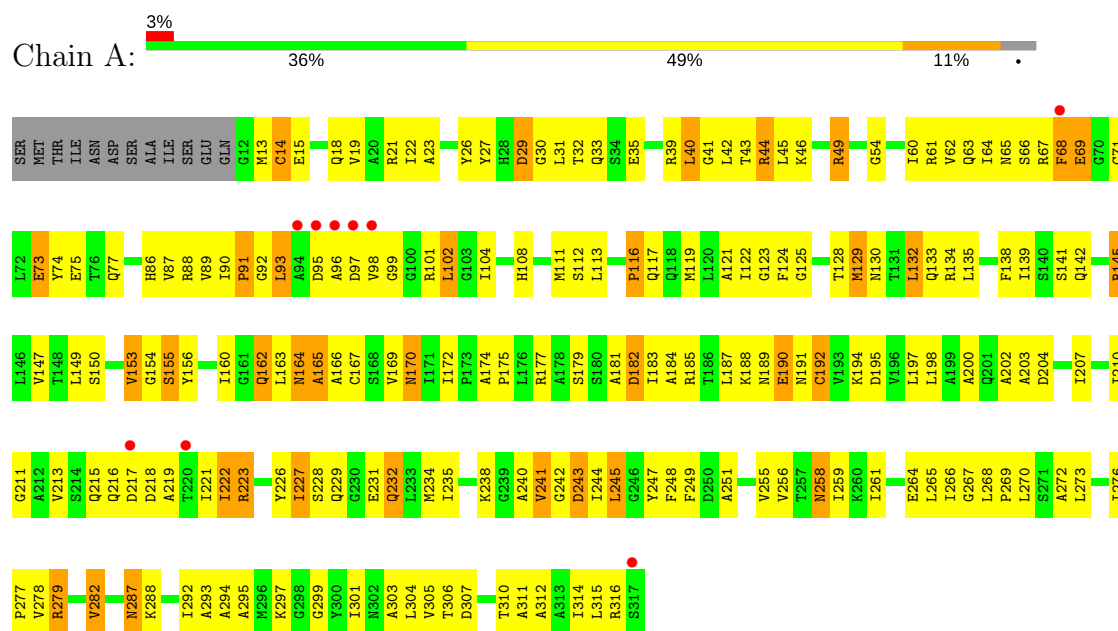
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P76141
B	0	SER	-	EXPRESSION TAG	UNP P76141
C	0	SER	-	EXPRESSION TAG	UNP P76141
D	0	SER	-	EXPRESSION TAG	UNP P76141

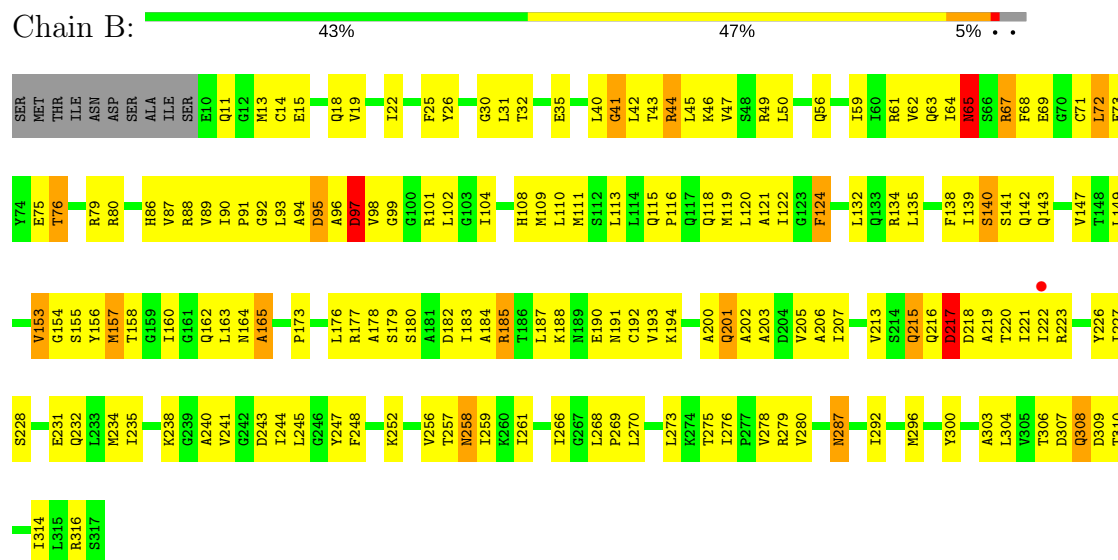
### 3 Residue-property plots

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.

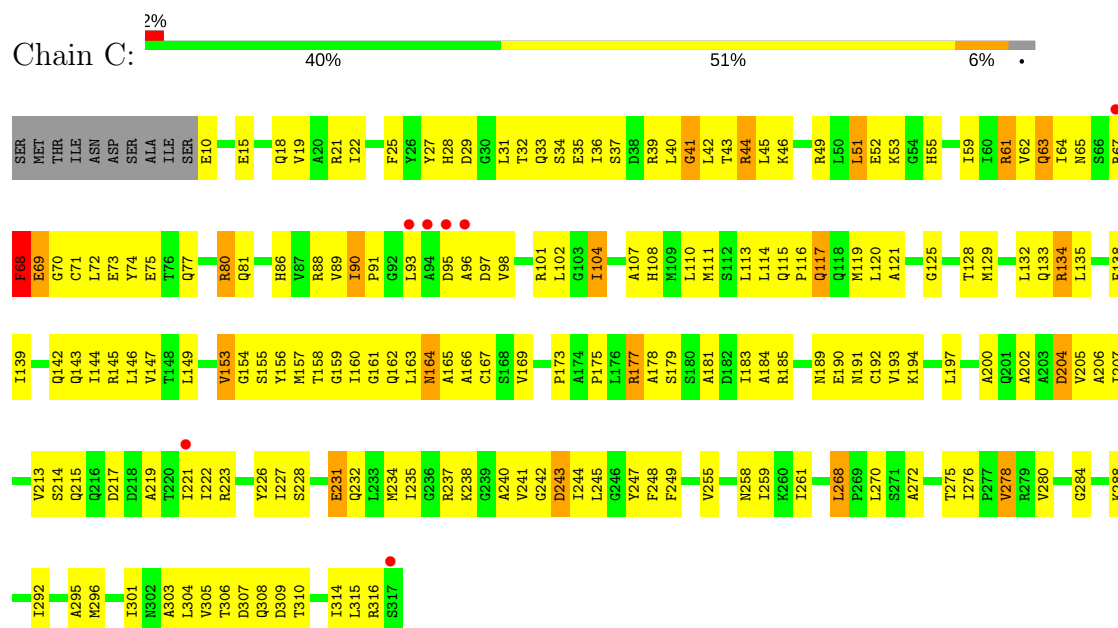
#### • Molecule 1: Transcriptional regulator LsrR



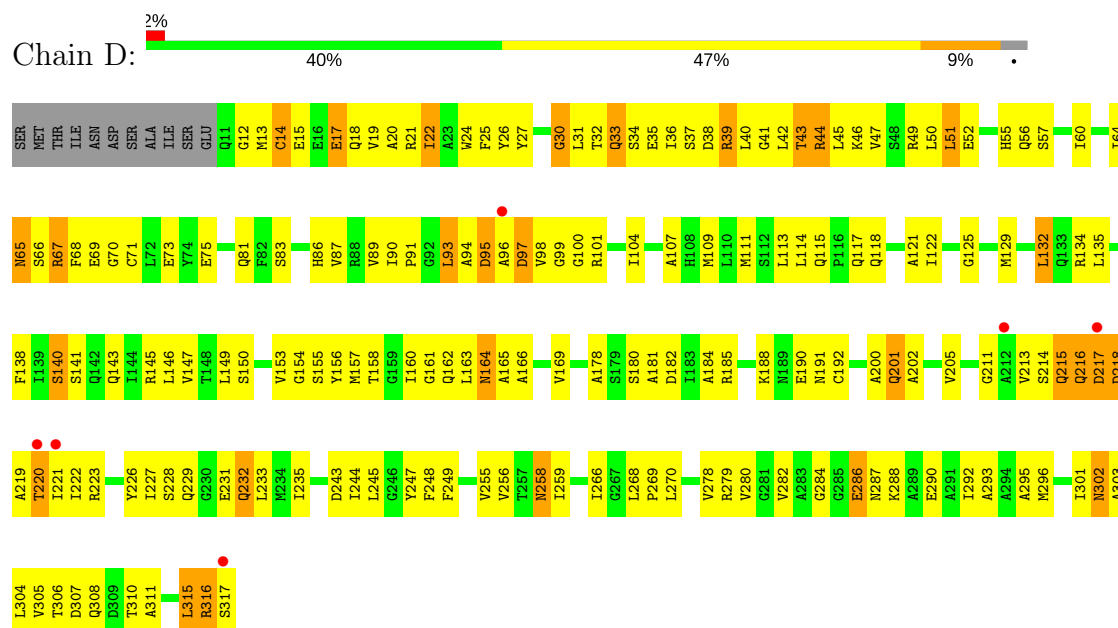
#### • Molecule 1: Transcriptional regulator LsrR



• Molecule 1: Transcriptional regulator LsrR



• Molecule 1: Transcriptional regulator LsrR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.74Å 80.53Å 103.64Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	47.98 – 3.21 47.98 – 3.21	Depositor EDS
% Data completeness (in resolution range)	89.2 (47.98-3.21) 89.3 (47.98-3.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.226 , 0.287 0.226 , 0.286	Depositor DCC
$R_{free}$ test set	1791 reflections (9.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.45	0/2312	0.67	0/3119
1	B	0.46	0/2330	0.65	0/3143
1	C	0.46	0/2330	0.67	0/3143
1	D	0.47	0/2321	0.67	0/3131
All	All	0.46	0/9293	0.66	0/12536

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2286	0	2340	220	0
1	B	2304	0	2354	193	0
1	C	2304	0	2354	196	0
1	D	2295	0	2348	190	0
All	All	9189	0	9396	760	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 41.

All (760) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:VAL:HG22	1:D:278:VAL:HB	1.42	0.99
1:B:231:GLU:O	1:B:235:ILE:HG12	1.68	0.94
1:B:43:THR:HG23	1:B:46:LYS:H	1.33	0.93
1:C:32:THR:HG22	1:C:34:SER:H	1.33	0.92
1:C:139:ILE:HG23	1:C:144:ILE:HB	1.51	0.92
1:A:13:MET:HG2	1:A:14:CYS:H	1.31	0.91
1:A:258:ASN:HD22	1:A:258:ASN:N	1.66	0.91
1:D:32:THR:HB	1:D:35:GLU:HG3	1.52	0.90
1:A:258:ASN:H	1:A:258:ASN:HD22	0.97	0.89
1:C:96:ALA:HB1	1:C:101:ARG:HD3	1.53	0.89
1:D:43:THR:HG23	1:D:46:LYS:HB2	1.55	0.88
1:B:268:LEU:HD12	1:B:269:PRO:HD2	1.54	0.88
1:C:32:THR:HG23	1:C:33:GLN:NE2	1.89	0.86
1:A:67:ARG:HB2	1:D:141:SER:HA	1.55	0.85
1:A:66:SER:HB3	1:A:69:GLU:HG2	1.58	0.85
1:A:43:THR:OG1	1:A:46:LYS:HG2	1.76	0.84
1:C:32:THR:HG23	1:C:33:GLN:HE21	1.42	0.83
1:C:238:LYS:HD2	1:C:258:ASN:OD1	1.77	0.83
1:C:221:ILE:HG13	1:C:227:ILE:HD13	1.60	0.82
1:D:21:ARG:HG3	1:D:25:PHE:HE2	1.43	0.82
1:B:243:ASP:HB3	1:B:248:PHE:CD1	2.14	0.82
1:A:207:ILE:HD11	1:A:282:VAL:HG12	1.61	0.81
1:B:44:ARG:H	1:B:44:ARG:HD2	1.44	0.81
1:B:93:LEU:HD13	1:C:29:ASP:OD1	1.81	0.81
1:A:258:ASN:ND2	1:A:258:ASN:H	1.73	0.81
1:C:71:CYS:O	1:C:75:GLU:HG3	1.79	0.81
1:A:238:LYS:HD3	1:A:258:ASN:OD1	1.80	0.80
1:A:111:MET:HG2	1:A:138:PHE:CD2	2.16	0.80
1:B:180:SER:HB3	1:B:183:ILE:HG13	1.63	0.80
1:D:104:ILE:H	1:D:104:ILE:HD12	1.45	0.80
1:C:80:ARG:HB2	1:C:80:ARG:NH1	1.97	0.79
1:C:226:TYR:C	1:C:227:ILE:HD12	2.03	0.78
1:D:284:GLY:O	1:D:288:LYS:HD3	1.83	0.78
1:D:21:ARG:HG3	1:D:25:PHE:CE2	2.17	0.78
1:C:74:TYR:HD1	1:C:315:LEU:HD12	1.49	0.77
1:A:153:VAL:HG21	1:B:173:PRO:HA	1.66	0.77
1:C:18:GLN:O	1:C:22:ILE:HG13	1.84	0.77
1:D:215:GLN:HB2	1:D:287:ASN:HD21	1.50	0.77
1:D:222:ILE:HD12	1:D:232:GLN:HG3	1.67	0.76
1:B:217:ASP:HA	1:B:222:ILE:HG21	1.68	0.76
1:A:170:ASN:N	1:A:170:ASN:HD22	1.84	0.76
1:A:102:LEU:HD13	1:A:282:VAL:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:HB2	1:D:161:GLY:O	1.87	0.75
1:C:32:THR:HB	1:C:35:GLU:HG3	1.67	0.75
1:C:51:LEU:HD23	1:C:52:GLU:N	2.01	0.75
1:D:157:MET:CE	1:D:160:ILE:HD11	2.18	0.74
1:D:279:ARG:H	1:D:302:ASN:HD21	1.34	0.74
1:C:205:VAL:HG13	1:C:278:VAL:HB	1.70	0.74
1:A:187:LEU:HD21	1:B:187:LEU:HD21	1.70	0.73
1:D:44:ARG:HD2	1:D:45:LEU:HD22	1.69	0.73
1:D:64:ILE:HB	1:D:69:GLU:HG3	1.69	0.73
1:B:279:ARG:HG3	1:B:279:ARG:HH11	1.54	0.73
1:C:149:LEU:HD23	1:C:200:ALA:HB1	1.70	0.73
1:C:231:GLU:O	1:C:235:ILE:HG13	1.87	0.73
1:B:32:THR:H	1:B:35:GLU:HG2	1.54	0.72
1:A:304:LEU:HD12	1:A:305:VAL:H	1.55	0.71
1:B:147:VAL:HG22	1:B:200:ALA:HB2	1.71	0.71
1:B:25:PHE:O	1:B:31:LEU:HD13	1.90	0.71
1:C:72:LEU:N	1:C:72:LEU:HD12	2.05	0.71
1:B:213:VAL:HG23	1:B:241:VAL:C	2.11	0.71
1:C:98:VAL:O	1:C:102:LEU:HD13	1.91	0.71
1:A:179:SER:HB3	1:B:190:GLU:OE2	1.90	0.70
1:A:221:ILE:HD12	1:A:226:TYR:HD2	1.55	0.70
1:A:292:ILE:O	1:A:295:ALA:HB3	1.91	0.70
1:B:234:MET:SD	1:B:238:LYS:HE2	2.31	0.70
1:C:189:ASN:ND2	1:C:194:LYS:NZ	2.39	0.70
1:B:121:ALA:HB1	1:B:149:LEU:HD21	1.72	0.70
1:D:235:ILE:CD1	1:D:259:ILE:HD12	2.22	0.69
1:C:89:VAL:HA	1:C:306:THR:O	1.92	0.69
1:C:119:MET:HE2	1:C:147:VAL:HG12	1.73	0.69
1:A:204:ASP:O	1:A:277:PRO:HG2	1.93	0.69
1:A:102:LEU:HD22	1:A:282:VAL:HG23	1.74	0.68
1:A:288:LYS:O	1:A:292:ILE:HG13	1.92	0.68
1:D:286:GLU:CD	1:D:286:GLU:H	1.96	0.68
1:A:61:ARG:NH1	1:A:62:VAL:H	1.91	0.68
1:B:185:ARG:HH11	1:B:185:ARG:HG2	1.59	0.68
1:C:72:LEU:HD12	1:C:72:LEU:H	1.58	0.68
1:D:184:ALA:HA	1:D:266:ILE:HD11	1.74	0.68
1:D:111:MET:HE3	1:D:138:PHE:HB2	1.74	0.68
1:D:229:GLN:H	1:D:229:GLN:CD	1.97	0.68
1:D:302:ASN:H	1:D:302:ASN:HD22	1.42	0.68
1:A:164:ASN:ND2	1:A:166:ALA:HB3	2.08	0.68
1:B:184:ALA:HA	1:B:266:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:H	1:B:35:GLU:CG	2.07	0.67
1:A:311:ALA:HA	1:A:314:ILE:HD12	1.77	0.67
1:D:25:PHE:O	1:D:31:LEU:HD23	1.93	0.67
1:D:243:ASP:HB3	1:D:248:PHE:CD1	2.30	0.67
1:D:293:ALA:HA	1:D:296:MET:HE3	1.74	0.67
1:B:227:ILE:HD13	1:B:261:ILE:HD12	1.76	0.67
1:B:67:ARG:HD3	1:B:68:PHE:CE2	2.30	0.67
1:A:247:TYR:CE2	1:A:269:PRO:HA	2.30	0.66
1:D:18:GLN:O	1:D:22:ILE:HG23	1.95	0.66
1:C:80:ARG:HB2	1:C:80:ARG:HH11	1.59	0.66
1:A:183:ILE:O	1:A:187:LEU:HG	1.94	0.66
1:B:64:ILE:HB	1:B:69:GLU:HG3	1.78	0.66
1:B:92:GLY:H	1:B:308:GLN:NE2	1.93	0.66
1:C:110:LEU:HD11	1:C:207:ILE:HD12	1.76	0.66
1:B:141:SER:HA	1:C:67:ARG:HB3	1.77	0.66
1:D:39:ARG:HE	1:D:39:ARG:HA	1.59	0.66
1:B:292:ILE:O	1:B:296:MET:HE2	1.95	0.66
1:C:189:ASN:ND2	1:C:194:LYS:HZ3	1.93	0.66
1:B:206:ALA:HB2	1:B:276:ILE:HD13	1.77	0.65
1:C:120:LEU:HD12	1:C:205:VAL:O	1.97	0.65
1:C:228:SER:OG	1:C:231:GLU:HB2	1.94	0.65
1:C:49:ARG:HD2	1:C:53:LYS:NZ	2.10	0.65
1:D:157:MET:HE2	1:D:160:ILE:HD11	1.79	0.65
1:A:102:LEU:CD1	1:A:282:VAL:HG23	2.26	0.65
1:B:247:TYR:CD2	1:B:270:LEU:HD13	2.32	0.65
1:B:141:SER:HB3	1:C:67:ARG:H	1.61	0.65
1:B:222:ILE:HG13	1:B:227:ILE:HG23	1.79	0.65
1:C:163:LEU:HD22	1:C:163:LEU:N	2.12	0.65
1:A:203:ALA:O	1:A:276:ILE:HG23	1.97	0.64
1:D:160:ILE:HA	1:D:163:LEU:HD11	1.78	0.64
1:B:40:LEU:HB2	1:B:42:LEU:HD13	1.80	0.64
1:B:219:ALA:C	1:B:221:ILE:H	2.01	0.64
1:C:221:ILE:CG1	1:C:227:ILE:HD13	2.27	0.64
1:C:67:ARG:O	1:C:68:PHE:HB3	1.96	0.64
1:D:44:ARG:HH11	1:D:45:LEU:CD2	2.11	0.64
1:A:33:GLN:HB2	1:A:44:ARG:NH1	2.12	0.64
1:B:134:ARG:HH11	1:B:134:ARG:HG2	1.62	0.64
1:A:67:ARG:O	1:A:68:PHE:HB2	1.97	0.64
1:D:91:PRO:O	1:D:101:ARG:NH2	2.31	0.64
1:B:184:ALA:O	1:B:188:LYS:HG3	1.97	0.64
1:D:140:SER:HB2	1:D:164:ASN:HD22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ILE:HD13	1:D:259:ILE:HD12	1.80	0.63
1:C:32:THR:HB	1:C:35:GLU:CG	2.28	0.63
1:A:160:ILE:HA	1:A:163:LEU:HD13	1.79	0.63
1:A:89:VAL:HA	1:A:306:THR:O	1.99	0.63
1:A:155:SER:OG	1:A:226:TYR:OH	2.14	0.63
1:A:207:ILE:HD11	1:A:282:VAL:CG1	2.29	0.63
1:A:119:MET:HB2	1:A:145:ARG:NH2	2.14	0.63
1:A:177:ARG:HB2	1:A:265:LEU:HD23	1.81	0.63
1:C:32:THR:HG22	1:C:34:SER:N	2.10	0.63
1:C:69:GLU:HA	1:C:72:LEU:HD13	1.81	0.63
1:D:215:GLN:HB2	1:D:287:ASN:ND2	2.12	0.63
1:A:29:ASP:OD2	1:D:93:LEU:HD21	1.99	0.63
1:C:75:GLU:OE2	1:C:88:ARG:HA	1.99	0.63
1:A:195:ASP:O	1:A:198:LEU:HB2	1.99	0.62
1:C:68:PHE:CG	1:C:68:PHE:O	2.52	0.62
1:A:155:SER:HG	1:A:226:TYR:HH	1.47	0.62
1:C:135:LEU:O	1:C:139:ILE:HG13	1.99	0.62
1:D:304:LEU:HD23	1:D:305:VAL:N	2.14	0.62
1:D:42:LEU:HD22	1:D:46:LYS:HB3	1.81	0.62
1:A:73:GLU:HG3	1:D:24:TRP:HH2	1.65	0.62
1:A:276:ILE:O	1:A:279:ARG:HD3	2.00	0.62
1:B:18:GLN:O	1:B:22:ILE:HG23	2.00	0.62
1:A:217:ASP:HB2	1:A:229:GLN:HE22	1.65	0.61
1:A:54:GLY:HA3	1:A:60:ILE:HD12	1.82	0.61
1:B:65:ASN:N	1:B:65:ASN:HD22	1.95	0.61
1:C:162:GLN:HG2	1:D:165:ALA:CB	2.30	0.61
1:D:157:MET:HE1	1:D:160:ILE:HD11	1.81	0.61
1:D:22:ILE:HG13	1:D:51:LEU:HD23	1.81	0.61
1:D:279:ARG:H	1:D:302:ASN:ND2	1.98	0.61
1:B:177:ARG:HH21	1:B:261:ILE:CD1	2.13	0.61
1:D:96:ALA:O	1:D:97:ASP:HB3	2.00	0.61
1:D:286:GLU:N	1:D:286:GLU:CD	2.52	0.61
1:C:139:ILE:HD12	1:C:163:LEU:HD11	1.82	0.61
1:C:179:SER:OG	1:C:183:ILE:HD12	2.00	0.61
1:D:44:ARG:HH11	1:D:45:LEU:HD21	1.64	0.61
1:C:153:VAL:O	1:C:156:TYR:HB2	2.01	0.61
1:C:165:ALA:HB2	1:D:161:GLY:C	2.21	0.61
1:A:221:ILE:CD1	1:A:226:TYR:HD2	2.13	0.61
1:A:222:ILE:O	1:A:222:ILE:HD13	2.01	0.61
1:B:232:GLN:O	1:B:235:ILE:HB	2.01	0.61
1:B:62:VAL:O	1:B:62:VAL:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASN:HD21	1:C:194:LYS:HZ3	1.47	0.60
1:D:38:ASP:O	1:D:39:ARG:HG2	2.00	0.60
1:B:279:ARG:HG3	1:B:279:ARG:NH1	2.15	0.60
1:D:213:VAL:O	1:D:216:GLN:HG3	2.01	0.60
1:A:21:ARG:HH22	1:D:70:GLY:C	2.05	0.60
1:D:140:SER:CB	1:D:164:ASN:ND2	2.64	0.60
1:B:141:SER:HA	1:C:67:ARG:CG	2.31	0.60
1:C:15:GLU:O	1:C:19:VAL:HG23	2.02	0.60
1:C:49:ARG:O	1:C:52:GLU:HG2	2.01	0.60
1:B:122:ILE:HD13	1:B:132:LEU:HD21	1.83	0.60
1:A:102:LEU:CD2	1:A:282:VAL:HG23	2.31	0.60
1:B:213:VAL:O	1:B:216:GLN:HG3	2.02	0.60
1:C:61:ARG:HE	1:C:62:VAL:N	1.99	0.60
1:A:73:GLU:HG3	1:D:24:TRP:CH2	2.36	0.60
1:A:147:VAL:HG11	1:A:200:ALA:HA	1.84	0.60
1:C:33:GLN:H	1:C:33:GLN:CD	2.04	0.60
1:D:44:ARG:CD	1:D:45:LEU:HD22	2.32	0.60
1:B:141:SER:HA	1:C:67:ARG:CB	2.32	0.59
1:C:70:GLY:O	1:C:73:GLU:HB3	2.02	0.59
1:D:39:ARG:HA	1:D:39:ARG:NE	2.17	0.59
1:D:15:GLU:O	1:D:19:VAL:HG23	2.02	0.59
1:A:217:ASP:HB2	1:A:229:GLN:NE2	2.16	0.59
1:D:67:ARG:HD2	1:D:68:PHE:CD2	2.38	0.59
1:C:154:GLY:C	1:C:156:TYR:H	2.06	0.59
1:C:36:ILE:O	1:C:39:ARG:HB3	2.03	0.59
1:A:39:ARG:HB3	1:A:40:LEU:HD12	1.83	0.59
1:B:96:ALA:O	1:B:97:ASP:HB3	2.01	0.59
1:B:179:SER:OG	1:B:183:ILE:HD12	2.02	0.59
1:B:292:ILE:HG22	1:B:296:MET:CE	2.31	0.59
1:B:43:THR:HG22	1:B:46:LYS:HB2	1.85	0.59
1:A:90:ILE:HD12	1:A:90:ILE:C	2.23	0.59
1:C:119:MET:HE2	1:C:147:VAL:CG1	2.33	0.59
1:B:79:ARG:NH1	1:B:87:VAL:HG12	2.18	0.59
1:B:97:ASP:CG	1:B:99:GLY:H	2.06	0.59
1:B:156:TYR:O	1:B:160:ILE:HG12	2.03	0.58
1:B:124:PHE:CE1	1:B:245:LEU:HD23	2.38	0.58
1:B:65:ASN:N	1:C:59:ILE:O	2.36	0.58
1:C:69:GLU:HA	1:C:72:LEU:CD1	2.33	0.58
1:A:124:PHE:HE1	1:A:245:LEU:HD23	1.67	0.58
1:B:141:SER:HB3	1:C:67:ARG:N	2.17	0.58
1:D:32:THR:HG22	1:D:34:SER:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ILE:O	1:C:301:ILE:HG13	2.04	0.58
1:D:140:SER:HB2	1:D:164:ASN:ND2	2.18	0.58
1:D:65:ASN:N	1:D:65:ASN:HD22	2.00	0.58
1:A:188:LYS:NZ	1:A:267:GLY:H	2.01	0.58
1:D:282:VAL:HG23	1:D:305:VAL:HB	1.85	0.58
1:C:189:ASN:HD22	1:C:194:LYS:HZ2	1.51	0.58
1:D:49:ARG:HH11	1:D:49:ARG:HG2	1.69	0.58
1:C:259:ILE:CG2	1:C:261:ILE:HG22	2.33	0.58
1:D:301:ILE:HG13	1:D:301:ILE:O	2.04	0.58
1:A:124:PHE:CE1	1:A:245:LEU:HD23	2.39	0.58
1:D:109:MET:HG2	1:D:113:LEU:HD11	1.85	0.58
1:B:235:ILE:HG22	1:B:240:ALA:HB3	1.86	0.57
1:D:232:GLN:O	1:D:235:ILE:HB	2.04	0.57
1:A:256:VAL:HB	1:A:259:ILE:HD12	1.87	0.57
1:C:177:ARG:NH1	1:C:261:ILE:HG13	2.19	0.57
1:C:310:THR:O	1:C:314:ILE:HG13	2.05	0.57
1:C:177:ARG:HD2	1:C:261:ILE:HG13	1.86	0.57
1:C:41:GLY:C	1:C:42:LEU:HD12	2.24	0.57
1:A:154:GLY:C	1:A:156:TYR:H	2.07	0.57
1:D:56:GLN:HA	1:D:134:ARG:HH11	1.70	0.57
1:B:147:VAL:CG2	1:B:200:ALA:HB2	2.34	0.57
1:B:65:ASN:N	1:B:65:ASN:ND2	2.53	0.57
1:B:62:VAL:HB	1:C:28:HIS:CE1	2.40	0.57
1:D:104:ILE:H	1:D:104:ILE:CD1	2.17	0.57
1:A:194:LYS:O	1:A:198:LEU:HD12	2.05	0.56
1:B:44:ARG:H	1:B:44:ARG:HH11	1.51	0.56
1:A:310:THR:O	1:A:314:ILE:HG13	2.04	0.56
1:A:27:TYR:HE2	1:A:60:ILE:HG21	1.69	0.56
1:C:213:VAL:HG23	1:C:241:VAL:C	2.25	0.56
1:A:29:ASP:OD2	1:D:93:LEU:HD11	2.05	0.56
1:B:32:THR:HG23	1:B:35:GLU:OE2	2.05	0.56
1:C:75:GLU:HG2	1:C:89:VAL:HG23	1.87	0.56
1:D:247:TYR:CD2	1:D:270:LEU:HD13	2.40	0.56
1:A:40:LEU:O	1:A:42:LEU:N	2.37	0.56
1:B:124:PHE:HE1	1:B:245:LEU:HD23	1.70	0.56
1:C:292:ILE:HG22	1:C:296:MET:HE2	1.88	0.56
1:D:33:GLN:HG3	1:D:34:SER:N	2.20	0.56
1:A:116:PRO:HG3	1:A:142:GLN:NE2	2.20	0.56
1:A:294:ALA:N	1:A:297:LYS:HE3	2.20	0.56
1:A:61:ARG:HA	1:A:61:ARG:CZ	2.35	0.56
1:B:160:ILE:HA	1:B:163:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASP:HA	1:B:222:ILE:CG2	2.35	0.56
1:C:121:ALA:HB1	1:C:149:LEU:HG	1.88	0.56
1:A:122:ILE:HG21	1:A:132:LEU:HD21	1.88	0.56
1:B:64:ILE:HA	1:C:59:ILE:O	2.05	0.56
1:A:54:GLY:HA3	1:A:60:ILE:CD1	2.36	0.56
1:D:93:LEU:HD21	1:D:101:ARG:NE	2.20	0.56
1:A:102:LEU:HD13	1:A:282:VAL:CG2	2.34	0.55
1:A:150:SER:C	1:A:172:ILE:HD12	2.26	0.55
1:A:293:ALA:O	1:A:297:LYS:HG3	2.06	0.55
1:C:44:ARG:HB3	1:C:45:LEU:HD22	1.87	0.55
1:C:86:HIS:CE1	1:C:113:LEU:HD21	2.42	0.55
1:A:62:VAL:HG21	1:D:27:TYR:CD1	2.41	0.55
1:A:177:ARG:HB2	1:A:265:LEU:CD2	2.37	0.55
1:B:44:ARG:N	1:B:44:ARG:HD2	2.20	0.55
1:C:61:ARG:NE	1:C:62:VAL:H	2.04	0.55
1:A:33:GLN:HB2	1:A:44:ARG:HH11	1.70	0.55
1:C:167:CYS:O	1:C:169:VAL:HG23	2.07	0.55
1:D:121:ALA:HB1	1:D:149:LEU:HD21	1.89	0.55
1:D:122:ILE:CD1	1:D:132:LEU:HD21	2.36	0.55
1:A:160:ILE:HA	1:A:163:LEU:CD1	2.36	0.55
1:C:304:LEU:HD12	1:C:305:VAL:H	1.72	0.55
1:D:219:ALA:C	1:D:221:ILE:H	2.09	0.55
1:B:287:ASN:OD1	1:B:287:ASN:N	2.40	0.55
1:D:93:LEU:HD23	1:D:101:ARG:CZ	2.37	0.55
1:A:96:ALA:HB1	1:A:101:ARG:HD3	1.88	0.55
1:A:187:LEU:CD2	1:B:187:LEU:HD21	2.36	0.55
1:A:189:ASN:HA	1:A:194:LYS:HE3	1.89	0.55
1:A:192:CYS:HA	1:A:195:ASP:OD2	2.07	0.55
1:A:68:PHE:CD2	1:A:91:PRO:HB2	2.42	0.55
1:C:164:ASN:OD1	1:C:166:ALA:HB3	2.07	0.55
1:D:122:ILE:HG13	1:D:122:ILE:O	2.07	0.54
1:D:200:ALA:C	1:D:202:ALA:H	2.11	0.54
1:B:113:LEU:HD13	1:B:278:VAL:HG11	1.89	0.54
1:B:124:PHE:N	1:B:124:PHE:CD1	2.75	0.54
1:B:280:VAL:HA	1:B:303:ALA:HB3	1.89	0.54
1:D:104:ILE:HD12	1:D:104:ILE:N	2.17	0.54
1:B:219:ALA:O	1:B:223:ARG:HG2	2.08	0.54
1:D:149:LEU:HD23	1:D:200:ALA:HB1	1.88	0.54
1:A:102:LEU:HD22	1:A:282:VAL:CG2	2.36	0.54
1:B:256:VAL:HB	1:B:259:ILE:HD12	1.89	0.54
1:D:52:GLU:O	1:D:56:GLN:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:O	1:A:133:GLN:HB2	2.07	0.54
1:A:101:ARG:HH11	1:A:101:ARG:HG3	1.72	0.54
1:A:268:LEU:HG	1:A:272:ALA:HB3	1.89	0.54
1:B:101:ARG:HA	1:B:104:ILE:HD12	1.90	0.54
1:C:119:MET:CE	1:C:147:VAL:HG12	2.38	0.54
1:C:61:ARG:HE	1:C:62:VAL:H	1.56	0.54
1:A:71:CYS:O	1:A:75:GLU:HB2	2.07	0.54
1:B:292:ILE:HG22	1:B:296:MET:HE1	1.89	0.54
1:C:215:GLN:O	1:C:232:GLN:NE2	2.35	0.54
1:B:190:GLU:O	1:B:192:CYS:N	2.41	0.53
1:C:235:ILE:HD13	1:C:248:PHE:CE2	2.43	0.53
1:C:197:LEU:HD22	1:C:268:LEU:HD12	1.90	0.53
1:B:141:SER:HA	1:C:67:ARG:HG2	1.90	0.53
1:A:26:TYR:O	1:A:30:GLY:HA2	2.09	0.53
1:A:122:ILE:CG2	1:A:132:LEU:HD21	2.38	0.53
1:C:222:ILE:HD12	1:C:232:GLN:OE1	2.08	0.53
1:C:67:ARG:O	1:C:68:PHE:CB	2.55	0.53
1:A:163:LEU:O	1:A:165:ALA:N	2.41	0.53
1:B:92:GLY:H	1:B:308:GLN:HE21	1.56	0.53
1:A:189:ASN:HA	1:A:194:LYS:CE	2.39	0.53
1:D:89:VAL:HA	1:D:306:THR:O	2.07	0.53
1:A:29:ASP:CG	1:D:93:LEU:HD21	2.29	0.53
1:A:22:ILE:C	1:A:22:ILE:HD12	2.29	0.53
1:A:256:VAL:HB	1:A:259:ILE:CD1	2.39	0.53
1:B:43:THR:O	1:B:47:VAL:HG23	2.07	0.53
1:B:32:THR:N	1:B:35:GLU:HG2	2.23	0.53
1:C:116:PRO:HG3	1:C:142:GLN:NE2	2.23	0.53
1:A:194:LYS:HA	1:A:197:LEU:HD12	1.91	0.53
1:C:119:MET:HE2	1:C:147:VAL:CB	2.39	0.53
1:C:135:LEU:HG	1:C:138:PHE:HB3	1.91	0.53
1:D:81:GLN:NE2	1:D:315:LEU:HD23	2.24	0.53
1:D:37:SER:OG	1:D:42:LEU:O	2.25	0.53
1:A:219:ALA:O	1:A:223:ARG:HG2	2.07	0.52
1:B:154:GLY:C	1:B:156:TYR:H	2.12	0.52
1:B:258:ASN:HD22	1:B:258:ASN:N	2.07	0.52
1:C:247:TYR:HB2	1:C:270:LEU:HD13	1.91	0.52
1:B:92:GLY:N	1:B:308:GLN:NE2	2.57	0.52
1:B:222:ILE:HG13	1:B:227:ILE:O	2.09	0.52
1:D:214:SER:C	1:D:216:GLN:H	2.13	0.52
1:B:121:ALA:HB1	1:B:149:LEU:CD2	2.39	0.52
1:B:25:PHE:HB3	1:B:31:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASP:OD1	1:B:96:ALA:N	2.26	0.52
1:C:121:ALA:HB1	1:C:149:LEU:CG	2.40	0.52
1:D:221:ILE:O	1:D:226:TYR:HE2	1.93	0.52
1:A:42:LEU:HD22	1:A:46:LYS:HB3	1.92	0.52
1:C:74:TYR:CD1	1:C:315:LEU:HD12	2.37	0.52
1:D:247:TYR:CG	1:D:270:LEU:HD13	2.45	0.52
1:B:178:ALA:HB3	1:B:184:ALA:HB2	1.91	0.52
1:B:201:GLN:NE2	1:B:275:THR:OG1	2.43	0.52
1:A:200:ALA:C	1:A:202:ALA:H	2.14	0.52
1:B:185:ARG:NH1	1:B:185:ARG:HG2	2.23	0.52
1:C:177:ARG:HH11	1:C:261:ILE:HG13	1.74	0.52
1:D:140:SER:OG	1:D:164:ASN:ND2	2.43	0.52
1:A:234:MET:O	1:A:238:LYS:HG3	2.10	0.51
1:A:45:LEU:C	1:A:45:LEU:HD13	2.30	0.51
1:C:234:MET:O	1:C:238:LYS:HG2	2.10	0.51
1:A:102:LEU:HD23	1:A:102:LEU:O	2.10	0.51
1:B:222:ILE:HB	1:B:232:GLN:HE22	1.75	0.51
1:C:117:GLN:HA	1:C:143:GLN:O	2.09	0.51
1:C:244:ILE:HG13	1:C:249:PHE:CE2	2.45	0.51
1:C:244:ILE:HG13	1:C:249:PHE:HE2	1.75	0.51
1:C:45:LEU:HD22	1:C:45:LEU:N	2.25	0.51
1:B:183:ILE:O	1:B:187:LEU:HG	2.10	0.51
1:B:279:ARG:HD2	1:B:300:TYR:O	2.10	0.51
1:B:32:THR:H	1:B:35:GLU:CD	2.13	0.51
1:D:56:GLN:O	1:D:134:ARG:HA	2.10	0.51
1:C:43:THR:O	1:C:46:LYS:N	2.43	0.51
1:D:147:VAL:HG22	1:D:200:ALA:HB2	1.92	0.51
1:B:111:MET:HG2	1:B:138:PHE:CD2	2.46	0.51
1:B:201:GLN:HG3	1:B:268:LEU:HD11	1.93	0.51
1:C:134:ARG:HG2	1:C:134:ARG:HH11	1.75	0.51
1:C:204:ASP:N	1:C:204:ASP:OD2	2.43	0.51
1:D:97:ASP:OD2	1:D:100:GLY:N	2.43	0.51
1:D:164:ASN:OD1	1:D:166:ALA:HB3	2.10	0.51
1:D:292:ILE:CG2	1:D:304:LEU:HD11	2.41	0.51
1:D:109:MET:CE	1:D:305:VAL:HG22	2.41	0.51
1:A:40:LEU:HD12	1:A:40:LEU:N	2.25	0.51
1:B:222:ILE:HD12	1:B:232:GLN:OE1	2.09	0.51
1:C:101:ARG:HG3	1:C:101:ARG:HH11	1.76	0.51
1:D:181:ALA:O	1:D:185:ARG:HG3	2.10	0.51
1:D:44:ARG:NH1	1:D:45:LEU:HD11	2.25	0.51
1:D:163:LEU:O	1:D:165:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:GLN:OE1	1:C:115:GLN:HA	2.11	0.51
1:B:62:VAL:HG21	1:C:27:TYR:HB3	1.93	0.51
1:D:56:GLN:HA	1:D:134:ARG:NH1	2.26	0.51
1:B:179:SER:HG	1:B:183:ILE:HD12	1.76	0.51
1:B:258:ASN:HD22	1:B:258:ASN:H	1.59	0.51
1:B:177:ARG:HH21	1:B:261:ILE:HD12	1.75	0.50
1:B:222:ILE:HB	1:B:232:GLN:NE2	2.26	0.50
1:D:145:ARG:C	1:D:146:LEU:HD12	2.31	0.50
1:A:98:VAL:HA	1:A:101:ARG:HB2	1.93	0.50
1:A:119:MET:HG2	1:A:203:ALA:HA	1.93	0.50
1:D:256:VAL:HG12	1:D:259:ILE:HG12	1.92	0.50
1:B:227:ILE:HD12	1:B:231:GLU:OE2	2.11	0.50
1:C:134:ARG:CG	1:C:134:ARG:HH11	2.24	0.50
1:B:163:LEU:O	1:B:165:ALA:N	2.44	0.50
1:D:222:ILE:HG13	1:D:227:ILE:O	2.12	0.50
1:A:88:ARG:HH21	1:D:13:MET:CE	2.25	0.50
1:A:97:ASP:O	1:A:99:GLY:N	2.42	0.50
1:B:134:ARG:HH11	1:B:134:ARG:CG	2.23	0.50
1:C:243:ASP:HB3	1:C:248:PHE:CD1	2.46	0.50
1:A:165:ALA:HB3	1:B:162:GLN:HE21	1.77	0.50
1:C:133:GLN:NE2	1:C:158:THR:O	2.41	0.50
1:C:32:THR:O	1:C:36:ILE:HG13	2.11	0.50
1:D:117:GLN:HA	1:D:143:GLN:O	2.12	0.50
1:C:21:ARG:HH11	1:C:21:ARG:HG3	1.75	0.50
1:D:229:GLN:CD	1:D:229:GLN:N	2.64	0.50
1:A:235:ILE:HD12	1:A:248:PHE:CD2	2.47	0.50
1:B:154:GLY:O	1:B:157:MET:HG2	2.12	0.50
1:C:129:MET:O	1:C:133:GLN:HG3	2.12	0.50
1:C:178:ALA:HB3	1:C:184:ALA:HB2	1.94	0.50
1:D:121:ALA:HA	1:D:147:VAL:HG13	1.93	0.50
1:D:270:LEU:N	1:D:270:LEU:HD12	2.26	0.50
1:C:69:GLU:OE2	1:C:70:GLY:N	2.45	0.49
1:D:30:GLY:C	1:D:31:LEU:HD22	2.32	0.49
1:A:170:ASN:ND2	1:A:170:ASN:N	2.57	0.49
1:B:44:ARG:N	1:B:44:ARG:HH11	2.10	0.49
1:C:42:LEU:HB3	1:C:46:LYS:HB3	1.92	0.49
1:D:182:ASP:HA	1:D:185:ARG:HE	1.77	0.49
1:D:244:ILE:O	1:D:245:LEU:HB2	2.11	0.49
1:A:32:THR:OG1	1:A:35:GLU:HB2	2.12	0.49
1:C:101:ARG:HA	1:C:104:ILE:HD11	1.95	0.49
1:C:157:MET:CE	1:C:160:ILE:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:CG2	1:D:200:ALA:HB2	2.42	0.49
1:D:43:THR:O	1:D:47:VAL:HG23	2.12	0.49
1:A:113:LEU:HD22	1:A:278:VAL:HG11	1.93	0.49
1:B:140:SER:O	1:B:143:GLN:HG3	2.12	0.49
1:B:216:GLN:O	1:B:218:ASP:N	2.46	0.49
1:B:31:LEU:HB3	1:B:35:GLU:HG3	1.93	0.49
1:C:73:GLU:HG3	1:C:77:GLN:NE2	2.28	0.49
1:D:290:GLU:HA	1:D:290:GLU:OE2	2.12	0.49
1:A:203:ALA:HB3	1:A:276:ILE:HD13	1.95	0.49
1:B:115:GLN:O	1:B:118:GLN:HG3	2.13	0.49
1:B:41:GLY:C	1:B:42:LEU:HD12	2.32	0.49
1:C:175:PRO:HB3	1:D:192:CYS:SG	2.52	0.49
1:C:27:TYR:OH	1:C:55:HIS:NE2	2.45	0.49
1:D:26:TYR:O	1:D:30:GLY:HA2	2.13	0.49
1:C:96:ALA:HB1	1:C:101:ARG:CD	2.35	0.49
1:A:211:GLY:O	1:A:243:ASP:N	2.42	0.49
1:A:22:ILE:HD12	1:A:23:ALA:N	2.28	0.49
1:A:304:LEU:HD12	1:A:305:VAL:N	2.26	0.49
1:B:177:ARG:HG2	1:B:178:ALA:N	2.28	0.49
1:B:71:CYS:O	1:B:75:GLU:HB2	2.12	0.49
1:A:15:GLU:O	1:A:19:VAL:HG23	2.12	0.48
1:B:222:ILE:HA	1:B:227:ILE:HG22	1.95	0.48
1:C:308:GLN:HG3	1:C:309:ASP:H	1.77	0.48
1:D:71:CYS:SG	1:D:308:GLN:NE2	2.86	0.48
1:A:14:CYS:O	1:A:18:GLN:HG3	2.12	0.48
1:A:61:ARG:HG3	1:A:61:ARG:HH11	1.79	0.48
1:A:90:ILE:HD12	1:A:91:PRO:O	2.12	0.48
1:B:67:ARG:HD3	1:B:68:PHE:CD2	2.48	0.48
1:A:170:ASN:H	1:A:170:ASN:HD22	1.60	0.48
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.79	0.48
1:A:43:THR:CB	1:A:46:LYS:HG2	2.43	0.48
1:A:43:THR:O	1:A:46:LYS:N	2.47	0.48
1:A:68:PHE:O	1:A:69:GLU:CD	2.51	0.48
1:C:163:LEU:CD2	1:C:163:LEU:N	2.76	0.48
1:D:220:THR:HA	1:D:223:ARG:HB3	1.95	0.48
1:A:68:PHE:O	1:A:69:GLU:OE2	2.32	0.48
1:D:222:ILE:HA	1:D:227:ILE:HG13	1.95	0.48
1:D:211:GLY:HA3	1:D:243:ASP:OD2	2.13	0.48
1:A:13:MET:HG2	1:A:14:CYS:N	2.13	0.48
1:A:68:PHE:HE2	1:A:93:LEU:H	1.62	0.48
1:A:135:LEU:O	1:A:139:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD12	1:A:90:ILE:O	2.13	0.48
1:B:32:THR:N	1:B:35:GLU:OE2	2.45	0.48
1:C:190:GLU:O	1:C:192:CYS:N	2.47	0.48
1:A:125:GLY:O	1:A:129:MET:HB2	2.14	0.48
1:A:251:ALA:O	1:A:297:LYS:HD2	2.13	0.48
1:B:26:TYR:O	1:B:30:GLY:HA2	2.13	0.48
1:B:96:ALA:O	1:B:97:ASP:CB	2.62	0.48
1:D:162:GLN:N	1:D:162:GLN:CD	2.67	0.48
1:D:200:ALA:O	1:D:202:ALA:N	2.47	0.48
1:B:194:LYS:O	1:B:194:LYS:HG2	2.14	0.48
1:C:284:GLY:O	1:C:288:LYS:HD2	2.13	0.48
1:A:145:ARG:HH11	1:A:145:ARG:HG2	1.78	0.47
1:A:200:ALA:C	1:A:202:ALA:N	2.66	0.47
1:B:56:GLN:O	1:B:134:ARG:HA	2.14	0.47
1:B:95:ASP:O	1:B:98:VAL:HG23	2.14	0.47
1:C:160:ILE:HA	1:C:163:LEU:HD23	1.96	0.47
1:D:122:ILE:HD13	1:D:132:LEU:HD21	1.95	0.47
1:A:227:ILE:HG12	1:A:228:SER:N	2.29	0.47
1:B:72:LEU:HD13	1:B:76:THR:OG1	2.15	0.47
1:A:13:MET:CG	1:A:14:CYS:H	2.11	0.47
1:A:213:VAL:HG23	1:A:242:GLY:N	2.28	0.47
1:C:147:VAL:HG11	1:C:200:ALA:HA	1.96	0.47
1:A:221:ILE:HD12	1:A:226:TYR:CD2	2.44	0.47
1:A:88:ARG:HH21	1:D:13:MET:HE3	1.79	0.47
1:B:247:TYR:CG	1:B:270:LEU:HD13	2.49	0.47
1:C:33:GLN:HG3	1:C:44:ARG:NH1	2.30	0.47
1:D:270:LEU:N	1:D:270:LEU:CD1	2.76	0.47
1:A:304:LEU:HD21	1:A:306:THR:CG2	2.44	0.47
1:B:61:ARG:HH21	1:B:63:GLN:HE22	1.62	0.47
1:D:228:SER:HB2	1:D:229:GLN:NE2	2.29	0.47
1:A:222:ILE:HG23	1:A:223:ARG:N	2.30	0.47
1:B:75:GLU:HG3	1:B:89:VAL:HG23	1.97	0.47
1:B:75:GLU:HG2	1:B:87:VAL:HG13	1.97	0.47
1:C:160:ILE:HA	1:C:163:LEU:CD2	2.45	0.47
1:C:244:ILE:O	1:C:245:LEU:HB2	2.14	0.47
1:D:64:ILE:O	1:D:66:SER:N	2.48	0.47
1:A:213:VAL:HG23	1:A:241:VAL:C	2.34	0.47
1:B:93:LEU:HD23	1:B:93:LEU:C	2.35	0.47
1:A:69:GLU:C	1:A:71:CYS:N	2.68	0.47
1:A:190:GLU:O	1:A:192:CYS:N	2.48	0.47
1:C:272:ALA:O	1:C:275:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HB3	1:C:42:LEU:HD13	1.97	0.47
1:A:184:ALA:HA	1:A:266:ILE:HD11	1.96	0.46
1:B:219:ALA:C	1:B:221:ILE:N	2.67	0.46
1:D:13:MET:SD	1:D:17:GLU:HG2	2.55	0.46
1:D:288:LYS:O	1:D:292:ILE:HG13	2.15	0.46
1:A:117:GLN:HG2	1:A:117:GLN:O	2.15	0.46
1:C:119:MET:HE2	1:C:147:VAL:HB	1.98	0.46
1:C:213:VAL:HG23	1:C:242:GLY:N	2.30	0.46
1:C:49:ARG:HD2	1:C:53:LYS:HZ1	1.80	0.46
1:A:102:LEU:CD2	1:A:102:LEU:O	2.64	0.46
1:C:96:ALA:O	1:C:101:ARG:HG2	2.16	0.46
1:D:154:GLY:C	1:D:156:TYR:H	2.18	0.46
1:D:190:GLU:O	1:D:192:CYS:N	2.48	0.46
1:A:304:LEU:HG	1:A:305:VAL:N	2.30	0.46
1:B:110:LEU:HD11	1:B:207:ILE:HD12	1.96	0.46
1:B:292:ILE:HG22	1:B:296:MET:HE2	1.96	0.46
1:C:235:ILE:HG23	1:C:259:ILE:CD1	2.46	0.46
1:C:219:ALA:O	1:C:223:ARG:HG2	2.16	0.46
1:C:90:ILE:O	1:C:307:ASP:HA	2.16	0.46
1:C:64:ILE:HD12	1:C:64:ILE:N	2.30	0.46
1:A:200:ALA:O	1:A:202:ALA:N	2.48	0.46
1:A:258:ASN:ND2	1:A:258:ASN:N	2.40	0.46
1:C:235:ILE:HG23	1:C:259:ILE:HD12	1.97	0.46
1:D:67:ARG:CZ	1:D:68:PHE:CE2	2.99	0.46
1:A:227:ILE:CG1	1:A:231:GLU:HB3	2.45	0.46
1:B:217:ASP:C	1:B:219:ALA:H	2.19	0.46
1:C:157:MET:HE2	1:C:160:ILE:HD11	1.98	0.46
1:C:206:ALA:HB2	1:C:276:ILE:HD13	1.98	0.46
1:B:134:ARG:CG	1:B:134:ARG:NH1	2.79	0.45
1:B:154:GLY:HA2	1:B:157:MET:CG	2.46	0.45
1:C:107:ALA:O	1:C:111:MET:HG3	2.16	0.45
1:C:72:LEU:CD1	1:C:72:LEU:N	2.75	0.45
1:D:307:ASP:OD1	1:D:310:THR:OG1	2.29	0.45
1:B:200:ALA:C	1:B:202:ALA:H	2.19	0.45
1:B:59:ILE:O	1:B:59:ILE:HG22	2.17	0.45
1:D:51:LEU:HA	1:D:51:LEU:HD22	1.72	0.45
1:A:279:ARG:HB2	1:A:279:ARG:HE	1.38	0.45
1:A:33:GLN:CB	1:A:44:ARG:NH1	2.80	0.45
1:A:75:GLU:HG3	1:A:87:VAL:HG12	1.98	0.45
1:A:87:VAL:HG12	1:A:88:ARG:N	2.31	0.45
1:B:124:PHE:CE1	1:B:245:LEU:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:SER:HB3	1:B:231:GLU:HB2	1.97	0.45
1:B:40:LEU:O	1:B:42:LEU:N	2.50	0.45
1:C:173:PRO:HG2	1:C:193:VAL:HG23	1.98	0.45
1:C:40:LEU:O	1:C:42:LEU:N	2.48	0.45
1:D:221:ILE:O	1:D:226:TYR:CE2	2.69	0.45
1:A:153:VAL:HG13	1:B:153:VAL:HG13	1.99	0.45
1:B:201:GLN:HG2	1:B:268:LEU:HD21	1.99	0.45
1:A:43:THR:HG23	1:A:46:LYS:HG2	1.98	0.45
1:A:27:TYR:CE2	1:A:60:ILE:HG21	2.51	0.45
1:A:61:ARG:NH1	1:A:62:VAL:N	2.60	0.45
1:C:132:LEU:HD11	1:C:146:LEU:HD21	1.98	0.45
1:A:95:ASP:O	1:A:96:ALA:HB3	2.15	0.45
1:A:165:ALA:CB	1:B:162:GLN:HE21	2.30	0.45
1:C:213:VAL:O	1:C:214:SER:C	2.53	0.45
1:D:200:ALA:C	1:D:202:ALA:N	2.70	0.45
1:A:147:VAL:HG23	1:A:170:ASN:HB2	1.98	0.45
1:A:222:ILE:C	1:A:222:ILE:HD13	2.37	0.45
1:A:287:ASN:N	1:A:287:ASN:OD1	2.47	0.45
1:A:63:GLN:HG3	1:A:64:ILE:N	2.32	0.45
1:B:116:PRO:HG3	1:B:142:GLN:HG3	1.98	0.45
1:B:67:ARG:H	1:B:67:ARG:HG3	1.50	0.45
1:A:104:ILE:HG12	1:A:134:ARG:NH2	2.31	0.45
1:A:45:LEU:O	1:A:49:ARG:HD2	2.17	0.45
1:C:104:ILE:HG23	1:C:134:ARG:CZ	2.46	0.45
1:C:40:LEU:HA	1:C:40:LEU:HD12	1.78	0.45
1:A:108:HIS:CE1	1:D:12:GLY:HA3	2.51	0.45
1:D:292:ILE:O	1:D:295:ALA:HB3	2.17	0.45
1:D:46:LYS:O	1:D:50:LEU:CD1	2.65	0.45
1:A:119:MET:HB2	1:A:145:ARG:HH21	1.79	0.45
1:A:150:SER:O	1:A:172:ILE:HD12	2.17	0.45
1:A:207:ILE:CD1	1:A:282:VAL:HG12	2.41	0.45
1:B:119:MET:HG2	1:B:203:ALA:CB	2.46	0.45
1:B:227:ILE:CD1	1:B:231:GLU:HB3	2.46	0.45
1:C:25:PHE:O	1:C:31:LEU:HD23	2.17	0.45
1:A:160:ILE:CA	1:A:163:LEU:HD13	2.45	0.45
1:A:164:ASN:HD22	1:A:166:ALA:HB3	1.81	0.45
1:A:43:THR:CG2	1:A:46:LYS:HG2	2.47	0.45
1:B:89:VAL:HA	1:B:306:THR:O	2.16	0.45
1:C:205:VAL:HG22	1:C:278:VAL:HG23	1.98	0.45
1:A:216:GLN:C	1:A:218:ASP:N	2.70	0.44
1:A:222:ILE:CG2	1:A:223:ARG:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:HD2	1:A:91:PRO:HB2	1.80	0.44
1:B:15:GLU:O	1:B:19:VAL:HG23	2.17	0.44
1:C:61:ARG:HH21	1:C:62:VAL:HB	1.81	0.44
1:B:93:LEU:HB3	1:B:101:ARG:NH1	2.33	0.44
1:A:194:LYS:HB2	1:A:194:LYS:HE3	1.80	0.44
1:A:261:ILE:HG12	1:A:261:ILE:O	2.16	0.44
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.71	0.44
1:A:294:ALA:HA	1:A:297:LYS:HE3	2.00	0.44
1:B:108:HIS:ND1	1:B:111:MET:HE3	2.31	0.44
1:D:122:ILE:HD12	1:D:132:LEU:HD21	2.00	0.44
1:D:228:SER:OG	1:D:231:GLU:HB2	2.17	0.44
1:B:122:ILE:HG13	1:B:122:ILE:O	2.17	0.44
1:B:49:ARG:HH11	1:B:49:ARG:HG3	1.83	0.44
1:B:80:ARG:HA	1:B:80:ARG:HD2	1.79	0.44
1:C:61:ARG:HA	1:C:61:ARG:NE	2.32	0.44
1:D:160:ILE:HA	1:D:163:LEU:CD1	2.47	0.44
1:A:244:ILE:HG13	1:A:249:PHE:HE2	1.83	0.44
1:C:200:ALA:C	1:C:202:ALA:H	2.21	0.44
1:C:95:ASP:O	1:C:96:ALA:HB3	2.17	0.44
1:D:115:GLN:HB2	1:D:118:GLN:OE1	2.17	0.44
1:A:77:GLN:HB3	1:A:315:LEU:CD1	2.47	0.44
1:D:40:LEU:O	1:D:42:LEU:N	2.51	0.44
1:A:227:ILE:HD11	1:A:232:GLN:HA	1.99	0.44
1:A:67:ARG:HH22	1:D:143:GLN:HB2	1.83	0.44
1:D:49:ARG:HH11	1:D:49:ARG:CG	2.30	0.44
1:D:98:VAL:HG12	1:D:98:VAL:O	2.18	0.44
1:A:108:HIS:NE2	1:D:12:GLY:HA3	2.33	0.44
1:A:90:ILE:O	1:A:307:ASP:HA	2.18	0.44
1:B:95:ASP:O	1:B:98:VAL:CG2	2.66	0.44
1:C:120:LEU:HD12	1:C:205:VAL:C	2.38	0.44
1:D:109:MET:HG2	1:D:113:LEU:CD1	2.48	0.44
1:D:95:ASP:HB2	1:D:96:ALA:H	1.64	0.44
1:A:182:ASP:O	1:A:185:ARG:HG2	2.18	0.44
1:A:279:ARG:NH2	1:A:299:GLY:O	2.50	0.44
1:B:65:ASN:ND2	1:B:65:ASN:H	2.14	0.44
1:C:80:ARG:CB	1:C:80:ARG:CZ	2.95	0.44
1:D:65:ASN:ND2	1:D:65:ASN:N	2.66	0.44
1:A:181:ALA:CA	1:A:264:GLU:HG2	2.48	0.43
1:A:29:ASP:HB3	1:A:31:LEU:HD13	2.00	0.43
1:B:157:MET:H	1:B:157:MET:HG2	1.59	0.43
1:B:215:GLN:O	1:B:219:ALA:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:CG1	1:B:307:ASP:OD2	2.66	0.43
1:C:121:ALA:O	1:C:206:ALA:HA	2.17	0.43
1:C:292:ILE:O	1:C:295:ALA:HB3	2.18	0.43
1:A:181:ALA:HA	1:A:264:GLU:HG2	2.00	0.43
1:A:67:ARG:HB2	1:D:141:SER:CA	2.39	0.43
1:D:227:ILE:HD12	1:D:232:GLN:HE21	1.83	0.43
1:A:215:GLN:HB2	1:A:219:ALA:HB2	2.00	0.43
1:B:86:HIS:HB3	1:B:109:MET:HE2	2.00	0.43
1:C:214:SER:OG	1:C:215:GLN:N	2.51	0.43
1:C:259:ILE:HG22	1:C:261:ILE:HG22	2.00	0.43
1:B:173:PRO:HG2	1:B:193:VAL:HG22	2.01	0.43
1:C:215:GLN:HB2	1:C:219:ALA:HB2	2.01	0.43
1:A:134:ARG:HD2	1:A:134:ARG:HA	1.87	0.43
1:A:240:ALA:HB1	1:A:248:PHE:HB3	2.00	0.43
1:B:268:LEU:CD1	1:B:269:PRO:HD2	2.38	0.43
1:D:93:LEU:CD2	1:D:101:ARG:CZ	2.95	0.43
1:A:304:LEU:CG	1:A:305:VAL:N	2.82	0.43
1:D:235:ILE:HD13	1:D:259:ILE:CD1	2.48	0.43
1:A:138:PHE:CE1	1:A:142:GLN:HG3	2.54	0.43
1:A:294:ALA:CA	1:A:297:LYS:HE3	2.48	0.43
1:B:44:ARG:CD	1:B:44:ARG:H	2.16	0.43
1:C:114:LEU:HD11	1:C:120:LEU:HD22	2.00	0.43
1:D:229:GLN:O	1:D:233:LEU:HG	2.19	0.43
1:D:311:ALA:O	1:D:315:LEU:HD12	2.18	0.43
1:D:32:THR:O	1:D:36:ILE:HG12	2.19	0.43
1:D:46:LYS:O	1:D:50:LEU:HD12	2.18	0.43
1:A:130:ASN:O	1:A:134:ARG:HG2	2.19	0.43
1:A:174:ALA:HB1	1:A:175:PRO:HD2	2.01	0.43
1:B:256:VAL:HB	1:B:259:ILE:CD1	2.48	0.43
1:C:280:VAL:HA	1:C:303:ALA:HB3	2.00	0.43
1:D:71:CYS:O	1:D:75:GLU:HB2	2.18	0.43
1:B:135:LEU:O	1:B:139:ILE:HG13	2.18	0.43
1:B:256:VAL:HG12	1:B:259:ILE:HG13	2.00	0.43
1:B:63:GLN:HB2	1:C:63:GLN:HE22	1.84	0.43
1:A:210:ILE:HD11	1:A:301:ILE:HD13	2.00	0.43
1:A:301:ILE:O	1:A:301:ILE:HG13	2.19	0.43
1:D:90:ILE:HA	1:D:91:PRO:HD3	1.91	0.43
1:A:304:LEU:HD21	1:A:306:THR:HG21	2.01	0.42
1:B:160:ILE:HA	1:B:163:LEU:CD1	2.49	0.42
1:B:227:ILE:HD11	1:B:231:GLU:HB3	2.00	0.42
1:B:90:ILE:HA	1:B:91:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ASP:HA	1:D:222:ILE:HG21	2.01	0.42
1:B:92:GLY:N	1:B:308:GLN:HE21	2.16	0.42
1:D:56:GLN:O	1:D:134:ARG:HD3	2.19	0.42
1:D:55:HIS:HD2	1:D:60:ILE:HB	1.84	0.42
1:C:104:ILE:O	1:C:108:HIS:HB2	2.19	0.42
1:C:121:ALA:HB1	1:C:149:LEU:HD21	2.00	0.42
1:D:147:VAL:HG11	1:D:200:ALA:HA	2.01	0.42
1:D:178:ALA:HB3	1:D:184:ALA:HB2	2.02	0.42
1:A:69:GLU:HG3	1:D:20:ALA:HB1	2.00	0.42
1:D:31:LEU:HD22	1:D:31:LEU:N	2.34	0.42
1:C:240:ALA:HA	1:C:249:PHE:O	2.19	0.42
1:D:214:SER:O	1:D:216:GLN:N	2.49	0.42
1:A:154:GLY:C	1:A:156:TYR:N	2.73	0.42
1:A:163:LEU:N	1:A:163:LEU:HD12	2.34	0.42
1:A:184:ALA:HA	1:A:266:ILE:CD1	2.50	0.42
1:A:244:ILE:HG13	1:A:249:PHE:CE2	2.55	0.42
1:B:176:LEU:HD12	1:B:176:LEU:O	2.20	0.42
1:D:114:LEU:HA	1:D:114:LEU:HD23	1.90	0.42
1:C:179:SER:OG	1:D:190:GLU:OE2	2.32	0.42
1:C:217:ASP:HA	1:C:222:ILE:HD13	2.02	0.42
1:D:215:GLN:O	1:D:219:ALA:HB2	2.20	0.42
1:D:36:ILE:CD1	1:D:47:VAL:HG11	2.49	0.42
1:B:227:ILE:HG13	1:B:231:GLU:HB3	2.01	0.42
1:B:87:VAL:HA	1:B:304:LEU:O	2.20	0.42
1:C:119:MET:CE	1:C:146:LEU:C	2.88	0.42
1:C:243:ASP:C	1:C:243:ASP:OD2	2.57	0.42
1:C:42:LEU:HD23	1:C:46:LYS:HD2	2.01	0.42
1:D:184:ALA:O	1:D:188:LYS:HG3	2.19	0.42
1:D:243:ASP:HB3	1:D:248:PHE:CE1	2.53	0.42
1:A:232:GLN:O	1:A:235:ILE:HB	2.20	0.42
1:B:235:ILE:HG22	1:B:240:ALA:CB	2.50	0.42
1:C:96:ALA:O	1:C:97:ASP:HB3	2.19	0.42
1:A:164:ASN:OD1	1:A:167:CYS:SG	2.78	0.42
1:B:219:ALA:O	1:B:221:ILE:N	2.53	0.42
1:C:101:ARG:O	1:C:104:ILE:HG12	2.20	0.42
1:D:146:LEU:N	1:D:146:LEU:HD12	2.35	0.42
1:D:216:GLN:O	1:D:218:ASP:N	2.53	0.42
1:A:160:ILE:HG22	1:A:163:LEU:CD2	2.49	0.42
1:A:238:LYS:HD3	1:A:258:ASN:CG	2.40	0.41
1:A:86:HIS:O	1:A:303:ALA:HA	2.20	0.41
1:B:310:THR:O	1:B:314:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:THR:HG22	1:D:33:GLN:N	2.34	0.41
1:C:207:ILE:HG23	1:C:207:ILE:O	2.21	0.41
1:C:43:THR:H	1:C:46:LYS:HB2	1.85	0.41
1:C:95:ASP:C	1:C:97:ASP:H	2.24	0.41
1:D:86:HIS:CD2	1:D:113:LEU:HD21	2.54	0.41
1:C:181:ALA:O	1:C:185:ARG:HG3	2.20	0.41
1:C:149:LEU:HD22	1:C:268:LEU:HD22	2.02	0.41
1:D:280:VAL:HA	1:D:303:ALA:HB3	2.03	0.41
1:B:102:LEU:HA	1:B:102:LEU:HD23	1.76	0.41
1:B:200:ALA:C	1:B:202:ALA:N	2.74	0.41
1:B:243:ASP:HB3	1:B:248:PHE:HD1	1.76	0.41
1:C:63:GLN:HB2	1:C:63:GLN:HE21	1.70	0.41
1:C:67:ARG:O	1:C:68:PHE:CD1	2.73	0.41
1:D:268:LEU:HA	1:D:269:PRO:HD3	1.77	0.41
1:A:134:ARG:NH1	1:A:134:ARG:HG3	2.36	0.41
1:C:119:MET:HE1	1:C:145:ARG:C	2.41	0.41
1:B:139:ILE:HD12	1:B:163:LEU:HD22	2.03	0.41
1:B:46:LYS:O	1:B:50:LEU:CD1	2.68	0.41
1:C:132:LEU:HA	1:C:132:LEU:HD13	1.87	0.41
1:D:316:ARG:HB3	1:D:317:SER:H	1.74	0.41
1:A:124:PHE:HA	1:A:129:MET:CE	2.50	0.41
1:B:252:LYS:HB3	1:B:252:LYS:NZ	2.35	0.41
1:C:121:ALA:HB1	1:C:149:LEU:CD2	2.51	0.41
1:C:159:GLY:C	1:C:161:GLY:H	2.23	0.41
1:D:219:ALA:C	1:D:221:ILE:N	2.73	0.41
1:D:217:ASP:C	1:D:219:ALA:H	2.23	0.41
1:A:121:ALA:HB1	1:A:149:LEU:HG	2.03	0.41
1:B:72:LEU:HA	1:B:72:LEU:HD22	1.87	0.41
1:D:125:GLY:O	1:D:129:MET:HB2	2.20	0.41
1:A:167:CYS:O	1:A:169:VAL:HG23	2.21	0.41
1:B:120:LEU:HD12	1:B:205:VAL:O	2.21	0.41
1:C:97:ASP:O	1:C:98:VAL:HB	2.21	0.41
1:D:216:GLN:HA	1:D:232:GLN:OE1	2.21	0.41
1:A:123:GLY:O	1:A:156:TYR:HE1	2.03	0.41
1:B:221:ILE:O	1:B:226:TYR:CE2	2.73	0.41
1:D:135:LEU:HA	1:D:135:LEU:HD12	1.88	0.41
1:D:36:ILE:HG13	1:D:47:VAL:HG11	2.03	0.41
1:A:132:LEU:HD13	1:A:132:LEU:HA	1.94	0.41
1:B:256:VAL:CG1	1:B:259:ILE:HG13	2.51	0.41
1:C:119:MET:HE1	1:C:146:LEU:N	2.36	0.41
1:C:81:GLN:O	1:C:81:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:VAL:O	1:D:282:VAL:HG13	2.22	0.41
1:D:40:LEU:HD12	1:D:40:LEU:HA	1.94	0.41
1:A:74:TYR:CE1	1:A:312:ALA:HA	2.57	0.40
1:B:244:ILE:O	1:B:244:ILE:HG22	2.21	0.40
1:C:205:VAL:HG22	1:C:278:VAL:CG2	2.51	0.40
1:C:21:ARG:NH1	1:C:21:ARG:HG3	2.36	0.40
1:D:247:TYR:N	1:D:247:TYR:CD1	2.90	0.40
1:A:75:GLU:OE2	1:A:88:ARG:HA	2.21	0.40
1:B:119:MET:HG2	1:B:203:ALA:HA	2.04	0.40
1:B:119:MET:CE	1:B:147:VAL:HB	2.52	0.40
1:D:107:ALA:O	1:D:111:MET:HG3	2.20	0.40
1:A:255:VAL:HG12	1:A:256:VAL:N	2.36	0.40
1:C:157:MET:C	1:C:159:GLY:H	2.25	0.40
1:D:147:VAL:HG21	1:D:200:ALA:N	2.36	0.40
1:A:231:GLU:O	1:A:235:ILE:HG12	2.20	0.40
1:B:104:ILE:HG12	1:B:134:ARG:HE	1.86	0.40
1:B:90:ILE:HG22	1:B:306:THR:O	2.22	0.40
1:B:46:LYS:O	1:B:50:LEU:HD13	2.22	0.40
1:C:125:GLY:O	1:C:129:MET:HB2	2.22	0.40
1:C:207:ILE:HA	1:C:280:VAL:O	2.21	0.40
1:D:255:VAL:HG12	1:D:256:VAL:N	2.36	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	304/318 (96%)	251 (83%)	39 (13%)	14 (5%)	3	21
1	B	306/318 (96%)	247 (81%)	40 (13%)	19 (6%)	2	13
1	C	306/318 (96%)	254 (83%)	44 (14%)	8 (3%)	6	37
1	D	305/318 (96%)	252 (83%)	33 (11%)	20 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1221/1272 (96%)	1004 (82%)	156 (13%)	61 (5%)	2	19

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	164	ASN
1	B	164	ASN
1	B	191	ASN
1	B	316	ARG
1	C	68	PHE
1	C	91	PRO
1	C	164	ASN
1	C	191	ASN
1	D	94	ALA
1	D	164	ASN
1	D	191	ASN
1	D	316	ARG
1	A	68	PHE
1	A	153	VAL
1	A	165	ALA
1	A	191	ASN
1	B	14	CYS
1	B	41	GLY
1	B	94	ALA
1	B	153	VAL
1	B	155	SER
1	C	93	LEU
1	C	153	VAL
1	D	14	CYS
1	D	153	VAL
1	D	201	GLN
1	A	41	GLY
1	A	192	CYS
1	B	11	GLN
1	B	65	ASN
1	B	73	GLU
1	B	140	SER
1	B	217	ASP
1	C	41	GLY
1	C	316	ARG
1	D	41	GLY

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Mol	Chain	Res	Type
1	D	65	ASN
1	D	140	SER
1	D	155	SER
1	D	215	GLN
1	D	218	ASP
1	A	14	CYS
1	A	93	LEU
1	A	155	SER
1	A	162	GLN
1	A	316	ARG
1	B	95	ASP
1	B	165	ALA
1	B	220	THR
1	D	39	ARG
1	D	258	ASN
1	B	13	MET
1	B	97	ASP
1	B	215	GLN
1	D	73	GLU
1	D	97	ASP
1	D	220	THR
1	A	92	GLY
1	D	30	GLY
1	D	99	GLY

### 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	238/249 (96%)	207 (87%)	31 (13%)	5	22
1	B	240/249 (96%)	219 (91%)	21 (9%)	12	42
1	C	240/249 (96%)	216 (90%)	24 (10%)	9	35
1	D	239/249 (96%)	212 (89%)	27 (11%)	7	29
All	All	957/996 (96%)	854 (89%)	103 (11%)	7	31

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	40	LEU
1	A	44	ARG
1	A	49	ARG
1	A	65	ASN
1	A	69	GLU
1	A	73	GLU
1	A	102	LEU
1	A	112	SER
1	A	116	PRO
1	A	128	THR
1	A	129	MET
1	A	132	LEU
1	A	141	SER
1	A	145	ARG
1	A	162	GLN
1	A	170	ASN
1	A	182	ASP
1	A	190	GLU
1	A	222	ILE
1	A	223	ARG
1	A	227	ILE
1	A	232	GLN
1	A	241	VAL
1	A	243	ASP
1	A	245	LEU
1	A	258	ASN
1	A	273	LEU
1	A	279	ARG
1	A	282	VAL
1	A	287	ASN
1	B	44	ARG
1	B	45	LEU
1	B	65	ASN
1	B	67	ARG
1	B	72	LEU
1	B	76	THR
1	B	88	ARG
1	B	97	ASP
1	B	124	PHE
1	B	157	MET
1	B	158	THR

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Mol	Chain	Res	Type
1	B	182	ASP
1	B	185	ARG
1	B	201	GLN
1	B	217	ASP
1	B	257	THR
1	B	258	ASN
1	B	273	LEU
1	B	287	ASN
1	B	308	GLN
1	B	309	ASP
1	C	10	GLU
1	C	37	SER
1	C	44	ARG
1	C	51	LEU
1	C	61	ARG
1	C	63	GLN
1	C	65	ASN
1	C	68	PHE
1	C	69	GLU
1	C	80	ARG
1	C	90	ILE
1	C	104	ILE
1	C	117	GLN
1	C	128	THR
1	C	134	ARG
1	C	155	SER
1	C	177	ARG
1	C	204	ASP
1	C	231	GLU
1	C	237	ARG
1	C	243	ASP
1	C	255	VAL
1	C	268	LEU
1	C	278	VAL
1	D	14	CYS
1	D	17	GLU
1	D	22	ILE
1	D	33	GLN
1	D	43	THR
1	D	44	ARG
1	D	51	LEU
1	D	57	SER

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Mol	Chain	Res	Type
1	D	67	ARG
1	D	83	SER
1	D	87	VAL
1	D	93	LEU
1	D	95	ASP
1	D	132	LEU
1	D	150	SER
1	D	158	THR
1	D	169	VAL
1	D	180	SER
1	D	201	GLN
1	D	216	GLN
1	D	217	ASP
1	D	232	GLN
1	D	249	PHE
1	D	258	ASN
1	D	286	GLU
1	D	302	ASN
1	D	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	65	ASN
1	A	117	GLN
1	A	130	ASN
1	A	142	GLN
1	A	170	ASN
1	A	232	GLN
1	A	258	ASN
1	B	11	GLN
1	B	33	GLN
1	B	63	GLN
1	B	65	ASN
1	B	162	GLN
1	B	201	GLN
1	B	308	GLN
1	C	28	HIS
1	C	33	GLN
1	C	63	GLN
1	C	65	ASN

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	86	HIS
1	C	117	GLN
1	C	130	ASN
1	C	164	ASN
1	C	189	ASN
1	C	216	GLN
1	D	65	ASN
1	D	81	GLN
1	D	130	ASN
1	D	143	GLN
1	D	164	ASN
1	D	201	GLN
1	D	215	GLN
1	D	216	GLN
1	D	229	GLN
1	D	287	ASN
1	D	302	ASN
1	D	308	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	306/318 (96%)	0.06	9 (2%)	52 38	36, 61, 103, 117	0
1	B	308/318 (96%)	-0.01	1 (0%)	93 92	37, 60, 102, 121	0
1	C	308/318 (96%)	0.03	7 (2%)	61 47	39, 60, 102, 117	0
1	D	307/318 (96%)	0.07	6 (1%)	65 51	38, 60, 100, 121	0
All	All	1229/1272 (96%)	0.04	23 (1%)	67 53	36, 61, 103, 121	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	ASP	6.1
1	C	94	ALA	5.3
1	A	94	ALA	3.9
1	D	317	SER	3.4
1	C	96	ALA	3.3
1	A	96	ALA	3.3
1	A	95	ASP	3.2
1	D	221	ILE	3.0
1	C	317	SER	2.9
1	B	222	ILE	2.7
1	A	217	ASP	2.6
1	A	317	SER	2.6
1	C	93	LEU	2.5
1	A	97	ASP	2.5
1	A	68	PHE	2.5
1	C	221	ILE	2.4
1	A	98	VAL	2.3
1	D	220	THR	2.3
1	C	67	ARG	2.2
1	A	220	THR	2.2
1	D	96	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	217	ASP	2.1
1	D	212	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.