



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:47 am BST

PDB ID : 2GK9  
Title : Human Phosphatidylinositol-4-phosphate 5-kinase, type II, gamma  
Authors : Uppenberg, J.; Hogbom, M.; Ogg, D.; Arrowsmith, C.; Berglund, H.; Collins, R.; Ehn, M.; Flodin, S.; Flores, A.; Graslund, S.; Holmberg-Schiavone, L.; Edwards, A.; Hammarstrom, M.; Kotenyova, T.; Nilsson-Ehle, P.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Hallberg, B.M.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-03-31  
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](mailto: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.

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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) : 1.13  
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

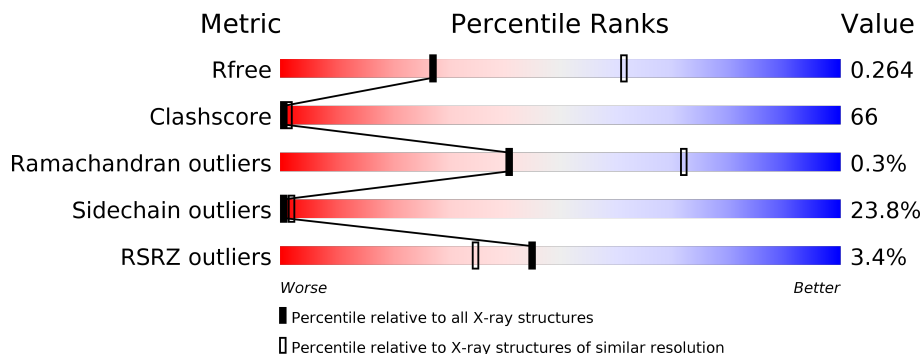
# 1 Overall quality at a glance

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  $\geq 3$ , 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	392	
1	B	392	
1	C	392	
1	D	392	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8233 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.

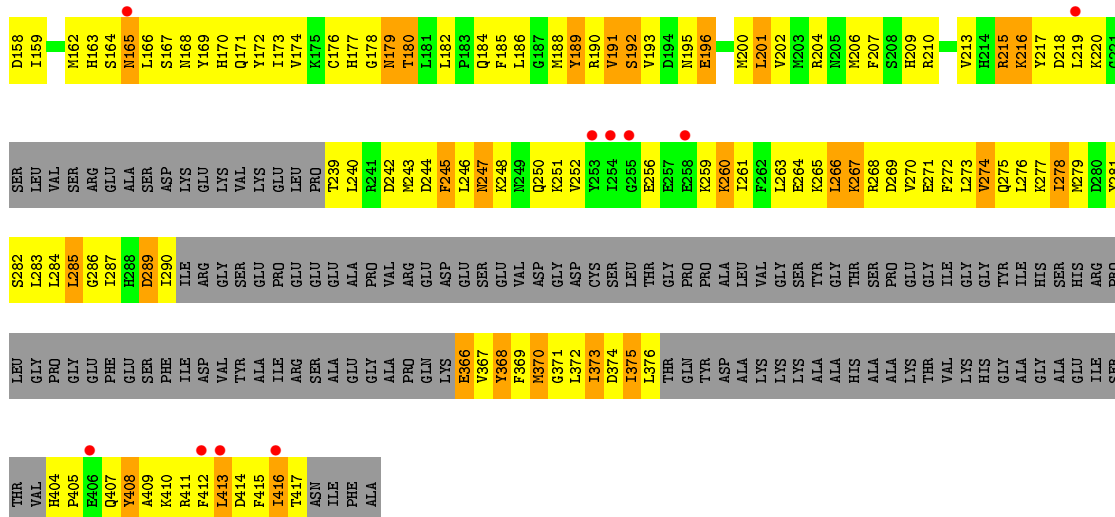
- Molecule 1 is a protein called phosphatidylinositol-4-phosphate 5-kinase, type II, gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	2023	1307	343	362	11	0	0	0
1	B	250	2084	1345	353	375	11	0	0	0
1	C	245	2042	1317	347	367	11	0	0	0
1	D	250	2084	1345	353	375	11	0	0	0

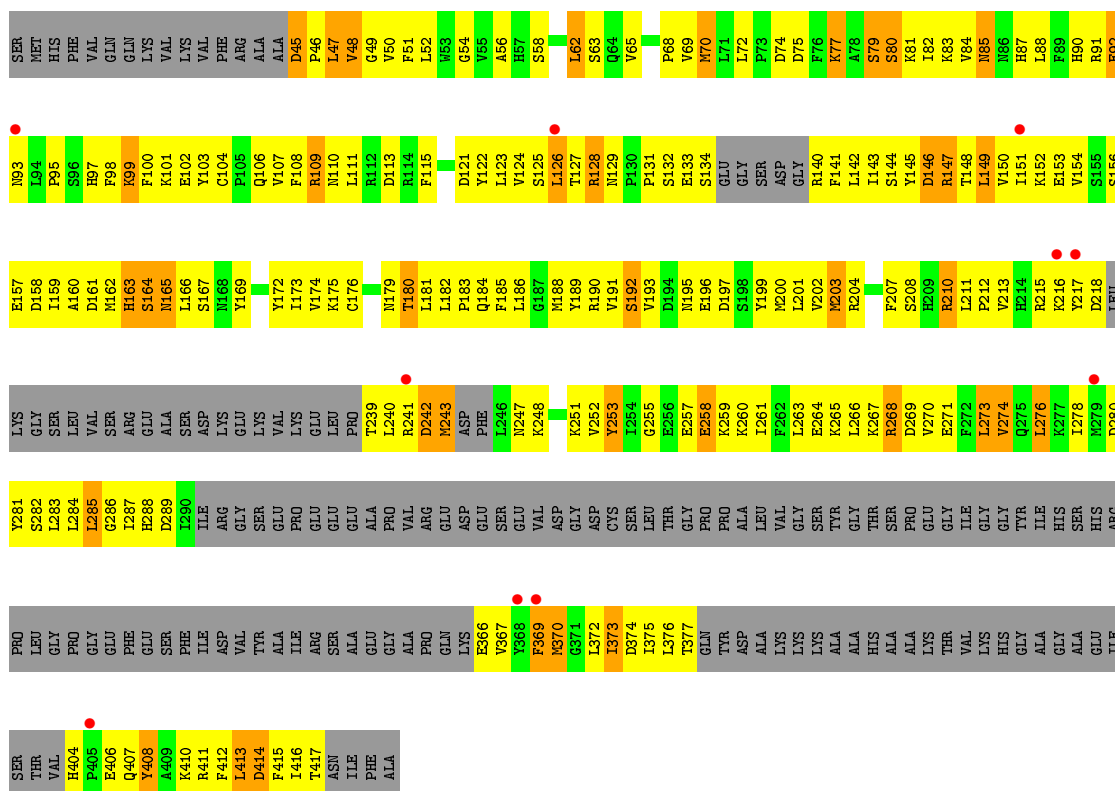
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	cloning artifact	UNP Q8TBX8
A	31	MET	-	cloning artifact	UNP Q8TBX8
B	30	SER	-	cloning artifact	UNP Q8TBX8
B	31	MET	-	cloning artifact	UNP Q8TBX8
C	30	SER	-	cloning artifact	UNP Q8TBX8
C	31	MET	-	cloning artifact	UNP Q8TBX8
D	30	SER	-	cloning artifact	UNP Q8TBX8
D	31	MET	-	cloning artifact	UNP Q8TBX8

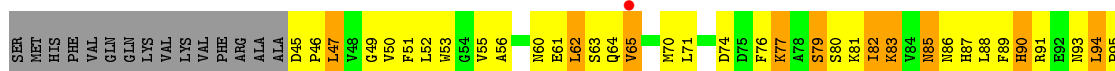


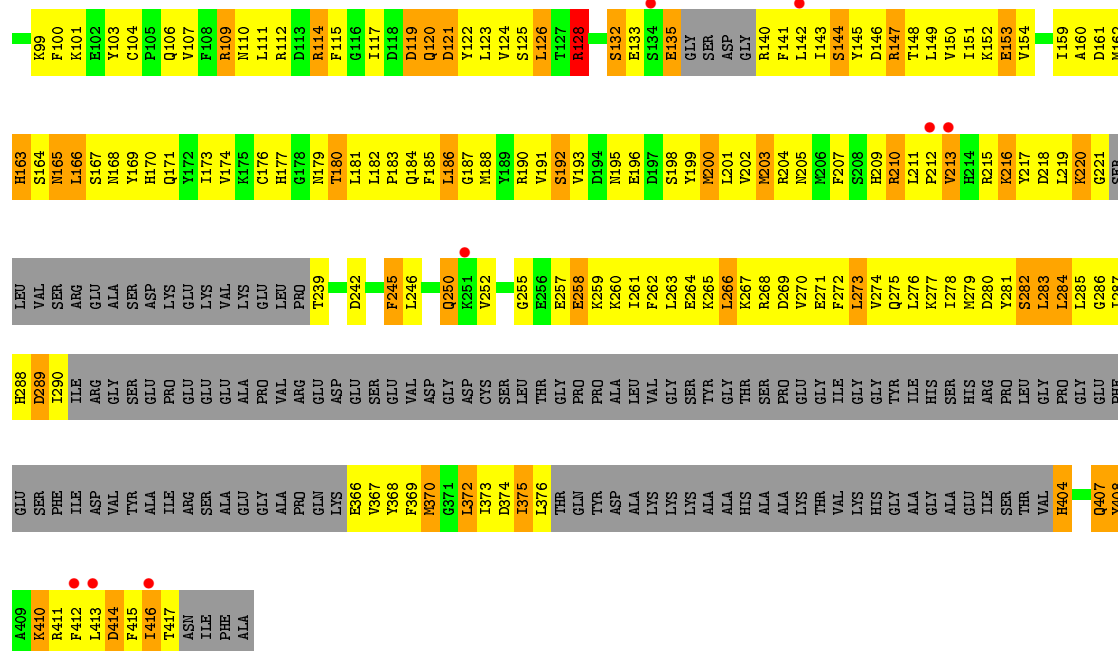


• Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma



• Molecule 1: phosphatidylinositol-4-phosphate 5-kinase, type II, gamma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.39Å 95.39Å 189.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.80) 95.5 (29.74-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.80Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.254 , 0.297 0.258 , 0.264	Depositor DCC
$R_{free}$ test set	1932 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 85.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [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	0.47	0/2068	0.58	4/2784 (0.1%)
1	B	0.47	0/2132	0.52	2/2872 (0.1%)
1	C	0.50	0/2088	0.58	5/2813 (0.2%)
1	D	0.45	0/2132	0.55	1/2872 (0.0%)
All	All	0.47	0/8420	0.56	12/11341 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	253	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	244	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	242	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	414	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	280	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	161	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	45	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	218	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	414	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	414	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	253	TYR	CB-CG-CD1	5.03	124.02	121.00



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	MET	Peptide
1	B	91	ARG	Peptide
1	D	128	ARG	Peptide

## 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	2023	0	2012	301	0
1	B	2084	0	2068	279	0
1	C	2042	0	2028	277	0
1	D	2084	0	2068	265	0
All	All	8233	0	8176	1077	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 66.

All (1077) 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:266:LEU:CD2	1:C:413:LEU:HD23	1.52	1.39
1:C:176:CYS:SG	1:C:180:THR:HG22	1.65	1.34
1:A:72:LEU:HD21	1:B:95:PRO:CA	1.64	1.25
1:A:72:LEU:CD2	1:B:95:PRO:HA	1.67	1.24
1:D:285:LEU:CD2	1:D:370:MET:HG2	1.66	1.24
1:C:266:LEU:HD23	1:C:413:LEU:CD2	1.68	1.24
1:D:285:LEU:HD23	1:D:370:MET:CG	1.69	1.21
1:D:215:ARG:HG2	1:D:215:ARG:HH11	1.13	1.12
1:B:266:LEU:HD22	1:B:413:LEU:HD23	1.24	1.12
1:D:220:LYS:HD2	1:D:282:SER:HB3	1.30	1.12
1:A:372:LEU:HD21	1:A:412:PHE:CZ	1.85	1.11
1:A:83:LYS:HD2	1:A:99:LYS:HD3	1.20	1.09
1:D:111:LEU:HD21	1:D:173:ILE:HG13	1.28	1.08
1:C:81:LYS:HD3	1:C:190:ARG:HH22	1.19	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:HD21	1:B:416:ILE:HD11	1.34	1.07
1:A:72:LEU:HG	1:A:73:PRO:HD2	1.33	1.06
1:C:266:LEU:HD23	1:C:413:LEU:HD23	1.07	1.05
1:D:141:PHE:CE1	1:D:152:LYS:HD2	1.89	1.05
1:B:140:ARG:HG3	1:B:153:GLU:HB3	1.39	1.04
1:D:285:LEU:HD23	1:D:370:MET:HG2	1.10	1.04
1:C:176:CYS:SG	1:C:180:THR:CG2	2.45	1.03
1:B:206:MET:CE	1:B:373:ILE:HG22	1.88	1.03
1:A:103:TYR:HB2	1:A:188:MET:HG2	1.40	1.02
1:C:266:LEU:HD22	1:C:413:LEU:HD23	1.42	1.01
1:D:285:LEU:HD23	1:D:370:MET:CB	1.89	1.01
1:B:126:LEU:HD12	1:B:151:ILE:HD11	1.39	1.01
1:D:111:LEU:CD2	1:D:173:ILE:HG13	1.90	1.01
1:A:266:LEU:CD2	1:A:413:LEU:HD23	1.90	1.01
1:A:47:LEU:HD12	1:A:191:VAL:HG22	1.41	1.01
1:B:283:LEU:HD21	1:B:370:MET:HE2	1.41	1.00
1:C:126:LEU:HD23	1:C:144:SER:HB2	1.45	0.99
1:C:270:VAL:HG11	1:C:413:LEU:HD11	1.45	0.97
1:A:417:THR:CG2	1:A:417:THR:O	2.10	0.97
1:B:83:LYS:HB3	1:C:83:LYS:HB3	1.46	0.97
1:A:417:THR:HG22	1:A:417:THR:O	1.63	0.96
1:B:206:MET:HE3	1:B:373:ILE:HG22	1.47	0.96
1:B:90:HIS:CE1	1:B:92:GLU:H	1.84	0.96
1:B:55:VAL:O	1:B:59:ILE:HG12	1.67	0.94
1:A:90:HIS:NE2	1:A:92:GLU:HB3	1.83	0.94
1:D:289:ASP:HB2	1:D:366:GLU:OE1	1.66	0.94
1:A:124:VAL:O	1:A:128:ARG:HB2	1.68	0.93
1:B:411:ARG:O	1:B:415:PHE:HB2	1.67	0.92
1:D:141:PHE:HE1	1:D:152:LYS:HD2	1.24	0.92
1:A:266:LEU:HD22	1:A:413:LEU:HD23	1.50	0.92
1:C:103:TYR:HB3	1:C:163:HIS:NE2	1.85	0.92
1:D:107:VAL:HG11	1:D:166:LEU:HD11	1.51	0.92
1:C:70:MET:HE3	1:D:46:PRO:HG3	1.49	0.91
1:D:372:LEU:HD12	1:D:372:LEU:H	1.33	0.91
1:C:404:HIS:HB2	1:C:407:GLN:HG3	1.49	0.91
1:D:124:VAL:HG23	1:D:128:ARG:HG3	1.53	0.91
1:C:140:ARG:HG2	1:C:153:GLU:HB3	1.50	0.90
1:A:372:LEU:HD21	1:A:412:PHE:CE2	2.06	0.90
1:B:90:HIS:HE1	1:B:92:GLU:HB3	1.34	0.90
1:D:192:SER:HA	1:D:196:GLU:O	1.69	0.90
1:A:52:LEU:HB3	1:A:127:THR:HG22	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HB3	1:B:190:ARG:HB3	1.50	0.90
1:C:52:LEU:HD23	1:C:127:THR:HA	1.55	0.89
1:B:412:PHE:CZ	1:B:416:ILE:HD13	2.08	0.88
1:A:281:TYR:HD1	1:A:372:LEU:HD11	1.38	0.86
1:B:285:LEU:HD22	1:B:286:GLY:H	1.40	0.86
1:C:80:SER:O	1:C:101:LYS:HA	1.73	0.86
1:D:285:LEU:HD23	1:D:370:MET:HB3	1.56	0.86
1:C:215:ARG:HD3	1:C:217:TYR:OH	1.75	0.86
1:D:258:GLU:HA	1:D:261:ILE:HD13	1.58	0.86
1:B:281:TYR:HA	1:B:374:ASP:HB3	1.59	0.85
1:C:257:GLU:O	1:C:261:ILE:HD12	1.76	0.85
1:D:169:TYR:CZ	1:D:173:ILE:HD11	2.11	0.85
1:A:213:VAL:HG23	1:A:287:ILE:H	1.42	0.84
1:B:271:GLU:O	1:B:275:GLN:HG3	1.77	0.84
1:C:267:LYS:HA	1:C:413:LEU:CD2	2.07	0.84
1:A:47:LEU:CD1	1:A:191:VAL:HG22	2.06	0.84
1:A:288:HIS:HB3	1:A:367:VAL:HB	1.59	0.83
1:A:372:LEU:CD2	1:A:412:PHE:CZ	2.60	0.83
1:D:257:GLU:O	1:D:261:ILE:HD12	1.78	0.83
1:D:273:LEU:HG	1:D:278:ILE:HD12	1.60	0.83
1:B:266:LEU:CD2	1:B:413:LEU:HD23	2.06	0.83
1:A:126:LEU:HD11	1:A:202:VAL:HG11	1.61	0.83
1:C:266:LEU:CD2	1:C:413:LEU:CD2	2.37	0.83
1:D:143:ILE:HG23	1:D:147:ARG:HA	1.60	0.82
1:B:283:LEU:HD21	1:B:370:MET:CE	2.09	0.82
1:A:407:GLN:OE1	1:A:407:GLN:HA	1.80	0.82
1:A:281:TYR:CD1	1:A:372:LEU:HD11	2.15	0.82
1:A:83:LYS:HD2	1:A:99:LYS:CD	2.08	0.82
1:A:217:TYR:H	1:A:285:LEU:HB3	1.44	0.82
1:A:74:ASP:HA	1:A:77:LYS:HE3	1.60	0.82
1:A:366:GLU:HB3	1:A:368:TYR:HE1	1.42	0.81
1:A:274:VAL:HG13	1:A:405:PRO:HB3	1.62	0.81
1:C:99:LYS:HB2	1:C:192:SER:HB2	1.62	0.81
1:B:412:PHE:CZ	1:B:416:ILE:CD1	2.63	0.81
1:A:46:PRO:O	1:A:50:VAL:HG23	1.80	0.81
1:B:273:LEU:HD12	1:B:278:ILE:HG21	1.63	0.81
1:D:124:VAL:CG2	1:D:128:ARG:HG3	2.10	0.80
1:D:218:ASP:OD1	1:D:282:SER:HB2	1.81	0.80
1:D:285:LEU:HD21	1:D:370:MET:HG2	1.62	0.80
1:C:373:ILE:HD13	1:C:374:ASP:N	1.97	0.80
1:D:74:ASP:HA	1:D:77:LYS:HG3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:CE1	1:A:184:GLN:HG2	2.17	0.80
1:A:134:SER:HB2	1:A:143:ILE:HD12	1.62	0.79
1:D:220:LYS:HD2	1:D:282:SER:CB	2.10	0.79
1:B:173:ILE:HG23	1:B:178:GLY:HA2	1.63	0.79
1:D:260:LYS:HE3	1:D:264:GLU:OE2	1.82	0.79
1:A:133:GLU:HA	1:A:142:LEU:HA	1.63	0.79
1:C:267:LYS:HA	1:C:413:LEU:HD22	1.62	0.79
1:C:103:TYR:HD1	1:C:188:MET:O	1.66	0.78
1:D:180:THR:OG1	1:D:182:LEU:HB2	1.82	0.78
1:A:279:MET:N	1:A:279:MET:SD	2.51	0.78
1:D:190:ARG:HD3	1:D:199:TYR:CE2	2.18	0.78
1:D:220:LYS:CD	1:D:282:SER:HB3	2.12	0.78
1:A:215:ARG:HB2	1:A:287:ILE:HD12	1.63	0.78
1:B:62:LEU:HD11	1:B:105:PRO:HB3	1.65	0.78
1:C:270:VAL:CG1	1:C:413:LEU:HD11	2.12	0.78
1:D:265:LYS:HG2	1:D:268:ARG:NH2	1.99	0.78
1:C:284:LEU:HB2	1:C:373:ILE:HG21	1.65	0.78
1:B:266:LEU:HD11	1:B:416:ILE:HG13	1.66	0.78
1:C:111:LEU:HD22	1:C:173:ILE:HD13	1.65	0.78
1:B:267:LYS:HG2	1:B:268:ARG:N	1.98	0.78
1:C:81:LYS:HD3	1:C:190:ARG:NH2	1.99	0.78
1:D:255:GLY:O	1:D:259:LYS:HB2	1.84	0.77
1:B:165:ASN:OD1	1:B:169:TYR:HB2	1.84	0.77
1:C:74:ASP:HA	1:C:77:LYS:HG3	1.67	0.77
1:A:72:LEU:HD11	1:B:95:PRO:HG3	1.66	0.77
1:B:286:GLY:O	1:B:368:TYR:HA	1.85	0.77
1:D:170:HIS:O	1:D:174:VAL:HG23	1.84	0.77
1:C:140:ARG:HG3	1:C:140:ARG:HH11	1.48	0.77
1:D:215:ARG:HG2	1:D:215:ARG:NH1	1.91	0.77
1:C:270:VAL:HG11	1:C:413:LEU:CD1	2.15	0.77
1:B:285:LEU:HD23	1:B:370:MET:HB3	1.65	0.76
1:C:255:GLY:HA3	1:C:258:GLU:OE2	1.84	0.76
1:C:288:HIS:O	1:C:366:GLU:HA	1.85	0.76
1:C:83:LYS:HD2	1:C:99:LYS:NZ	2.00	0.76
1:D:417:THR:O	1:D:417:THR:HG22	1.84	0.76
1:A:90:HIS:CD2	1:A:92:GLU:H	2.03	0.76
1:C:285:LEU:HD12	1:C:370:MET:HG2	1.67	0.76
1:D:81:LYS:HD3	1:D:101:LYS:HE3	1.66	0.76
1:B:215:ARG:HB2	1:B:287:ILE:HB	1.68	0.76
1:B:417:THR:O	1:B:417:THR:HG22	1.85	0.76
1:A:72:LEU:HG	1:A:73:PRO:CD	2.12	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TYR:HB3	1:A:219:LEU:HD21	1.68	0.76
1:C:162:MET:O	1:C:166:LEU:HB2	1.85	0.76
1:D:261:ILE:HA	1:D:264:GLU:OE1	1.85	0.76
1:C:126:LEU:CD2	1:C:144:SER:HB2	2.15	0.75
1:B:259:LYS:O	1:B:263:LEU:HG	1.86	0.75
1:C:126:LEU:HD11	1:C:151:ILE:HD11	1.68	0.75
1:D:80:SER:O	1:D:101:LYS:HA	1.86	0.75
1:A:259:LYS:O	1:A:263:LEU:HD12	1.85	0.75
1:A:276:LEU:HD12	1:A:278:ILE:HD11	1.68	0.75
1:D:261:ILE:H	1:D:261:ILE:HD12	1.52	0.75
1:C:287:ILE:HA	1:C:367:VAL:O	1.85	0.75
1:A:62:LEU:HD12	1:D:89:PHE:HZ	1.51	0.75
1:D:266:LEU:HD22	1:D:413:LEU:HD23	1.67	0.75
1:A:154:VAL:O	1:A:199:TYR:HB2	1.86	0.74
1:B:80:SER:O	1:B:101:LYS:HA	1.87	0.74
1:D:372:LEU:HD12	1:D:372:LEU:N	2.02	0.74
1:C:411:ARG:O	1:C:415:PHE:HB2	1.87	0.74
1:D:133:GLU:HA	1:D:142:LEU:HD23	1.68	0.74
1:A:151:ILE:HG23	1:A:202:VAL:HG22	1.69	0.74
1:B:90:HIS:CE1	1:B:92:GLU:HB3	2.18	0.74
1:A:62:LEU:HD23	1:A:109:ARG:NE	2.03	0.74
1:B:217:TYR:CE2	1:B:240:LEU:HD12	2.22	0.74
1:B:94:LEU:HD12	1:B:98:PHE:CE1	2.22	0.74
1:D:65:VAL:HG12	1:D:109:ARG:HH22	1.53	0.74
1:A:404:HIS:HD2	1:A:407:GLN:HG2	1.50	0.74
1:C:45:ASP:HB3	1:C:48:VAL:HG12	1.68	0.74
1:B:83:LYS:HD2	1:C:83:LYS:HD3	1.70	0.73
1:B:107:VAL:HG12	1:B:111:LEU:HD12	1.70	0.73
1:D:122:TYR:O	1:D:126:LEU:HB2	1.88	0.73
1:B:90:HIS:HE1	1:B:92:GLU:CB	2.02	0.73
1:A:165:ASN:O	1:A:169:TYR:CB	2.37	0.73
1:A:180:THR:HB	1:A:269:ASP:OD1	1.89	0.73
1:A:72:LEU:O	1:A:75:ASP:HB2	1.89	0.73
1:C:184:GLN:OE1	1:C:204:ARG:HD2	1.89	0.73
1:C:270:VAL:HG21	1:C:413:LEU:HG	1.70	0.73
1:C:70:MET:CE	1:D:46:PRO:HG3	2.17	0.73
1:A:59:ILE:HG21	1:A:123:LEU:HB2	1.70	0.72
1:B:171:GLN:O	1:B:174:VAL:HB	1.89	0.72
1:B:90:HIS:ND1	1:B:91:ARG:N	2.36	0.72
1:A:412:PHE:CE1	1:A:416:ILE:HG21	2.23	0.72
1:B:372:LEU:H	1:B:372:LEU:HD12	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:PHE:CE1	1:B:416:ILE:HD13	2.24	0.72
1:B:48:VAL:O	1:B:51:PHE:HB3	1.89	0.72
1:C:108:PHE:HB3	1:C:186:LEU:O	1.90	0.72
1:C:70:MET:HE2	1:D:93:ASN:O	1.90	0.72
1:B:99:LYS:HB2	1:B:192:SER:HB2	1.72	0.72
1:C:273:LEU:HD11	1:C:281:TYR:CE2	2.24	0.72
1:A:165:ASN:O	1:A:169:TYR:HB3	1.90	0.72
1:A:48:VAL:O	1:A:51:PHE:HB3	1.90	0.72
1:C:273:LEU:HA	1:C:278:ILE:HD12	1.71	0.71
1:A:272:PHE:HA	1:A:275:GLN:OE1	1.89	0.71
1:B:412:PHE:O	1:B:415:PHE:N	2.24	0.71
1:D:89:PHE:O	1:D:91:ARG:HG3	1.90	0.71
1:A:270:VAL:O	1:A:274:VAL:HG23	1.91	0.71
1:B:117:ILE:HD12	1:B:186:LEU:HD22	1.72	0.71
1:A:215:ARG:CB	1:A:287:ILE:HD12	2.20	0.71
1:D:65:VAL:HG12	1:D:109:ARG:NH2	2.06	0.71
1:D:372:LEU:CD1	1:D:372:LEU:H	2.02	0.71
1:A:266:LEU:HD23	1:A:413:LEU:HD23	1.72	0.71
1:C:124:VAL:HG23	1:C:128:ARG:HD3	1.73	0.70
1:C:85:ASN:HB3	1:C:97:HIS:NE2	2.06	0.70
1:C:273:LEU:HD12	1:C:278:ILE:CG2	2.21	0.70
1:B:52:LEU:HD22	1:B:126:LEU:O	1.92	0.70
1:A:90:HIS:NE2	1:A:92:GLU:CB	2.54	0.70
1:D:283:LEU:CD1	1:D:412:PHE:HZ	2.04	0.70
1:A:53:TRP:HB2	1:A:94:LEU:HD11	1.74	0.70
1:B:372:LEU:N	1:B:372:LEU:HD12	2.07	0.70
1:B:265:LYS:HG2	1:B:268:ARG:HH21	1.57	0.69
1:D:212:PRO:HD2	1:D:288:HIS:CE1	2.27	0.69
1:A:240:LEU:N	1:A:240:LEU:HD23	2.07	0.69
1:C:126:LEU:HD23	1:C:144:SER:CB	2.22	0.69
1:C:412:PHE:CE1	1:C:416:ILE:HD12	2.27	0.69
1:A:375:ILE:O	1:A:376:LEU:HD12	1.91	0.69
1:D:210:ARG:HG3	1:D:211:LEU:HD23	1.72	0.69
1:A:49:GLY:HA2	1:A:52:LEU:HD12	1.74	0.69
1:B:269:ASP:O	1:B:272:PHE:HB3	1.91	0.69
1:B:284:LEU:O	1:B:370:MET:HA	1.91	0.69
1:A:281:TYR:CB	1:A:374:ASP:O	2.40	0.69
1:A:134:SER:CB	1:A:143:ILE:HD12	2.23	0.69
1:A:173:ILE:HG23	1:A:178:GLY:HA2	1.74	0.69
1:A:51:PHE:HE2	1:A:151:ILE:HD13	1.57	0.69
1:A:273:LEU:HD23	1:A:278:ILE:HB	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:PHE:HD2	1:D:166:LEU:HD21	1.56	0.68
1:A:413:LEU:HA	1:A:416:ILE:CD1	2.23	0.68
1:D:259:LYS:O	1:D:263:LEU:HD12	1.93	0.68
1:A:240:LEU:H	1:A:240:LEU:HD23	1.58	0.68
1:B:59:ILE:CB	1:B:123:LEU:HD13	2.24	0.68
1:A:281:TYR:HB3	1:A:374:ASP:O	1.94	0.68
1:C:81:LYS:CD	1:C:190:ARG:HH22	2.01	0.68
1:C:266:LEU:HD23	1:C:413:LEU:HD21	1.74	0.68
1:B:273:LEU:HB2	1:B:278:ILE:HD12	1.76	0.68
1:D:110:ASN:O	1:D:114:ARG:HD3	1.94	0.68
1:A:220:LYS:HD2	1:A:280:ASP:OD1	1.94	0.68
1:D:47:LEU:HD12	1:D:191:VAL:HG12	1.74	0.68
1:A:107:VAL:HG11	1:A:166:LEU:HD21	1.76	0.67
1:B:141:PHE:CE1	1:B:152:LYS:HB2	2.29	0.67
1:A:62:LEU:HD23	1:A:109:ARG:HE	1.57	0.67
1:C:284:LEU:O	1:C:370:MET:HA	1.93	0.67
1:A:372:LEU:CD2	1:A:412:PHE:HZ	2.05	0.67
1:C:257:GLU:O	1:C:261:ILE:CD1	2.42	0.67
1:A:288:HIS:ND1	1:A:367:VAL:HG21	2.10	0.67
1:D:188:MET:HG3	1:D:201:LEU:HD12	1.74	0.67
1:B:217:TYR:HE2	1:B:240:LEU:HD12	1.59	0.67
1:A:404:HIS:CD2	1:A:407:GLN:HG2	2.29	0.67
1:D:215:ARG:CG	1:D:215:ARG:HH11	1.96	0.67
1:D:55:VAL:HG11	1:D:126:LEU:HD12	1.75	0.67
1:C:140:ARG:HG3	1:C:140:ARG:NH1	2.08	0.67
1:C:273:LEU:HD12	1:C:278:ILE:HG22	1.76	0.67
1:A:59:ILE:HD13	1:A:123:LEU:HB2	1.77	0.67
1:B:103:TYR:HB2	1:B:188:MET:HG2	1.75	0.67
1:C:404:HIS:HB2	1:C:407:GLN:CG	2.23	0.67
1:C:102:GLU:HG3	1:C:189:TYR:CD2	2.30	0.67
1:A:62:LEU:HD21	1:A:109:ARG:HB2	1.76	0.66
1:A:412:PHE:CZ	1:A:416:ILE:HD12	2.30	0.66
1:B:144:SER:HB3	1:B:149:LEU:O	1.96	0.66
1:C:266:LEU:O	1:C:270:VAL:N	2.24	0.66
1:A:106:GLN:O	1:A:109:ARG:HB3	1.95	0.66
1:A:373:ILE:HG12	1:A:374:ASP:N	2.11	0.66
1:B:154:VAL:HB	1:B:158:ASP:OD2	1.95	0.66
1:C:165:ASN:HB2	1:C:276:LEU:HD22	1.77	0.66
1:A:85:ASN:OD1	1:A:97:HIS:HA	1.95	0.66
1:C:265:LYS:HG2	1:C:268:ARG:NH2	2.10	0.66
1:B:103:TYR:CD1	1:B:188:MET:HG2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:O	1:A:82:ILE:HD13	1.94	0.66
1:C:213:VAL:HG22	1:C:369:PHE:CE2	2.31	0.66
1:B:59:ILE:HB	1:B:123:LEU:HD13	1.78	0.65
1:C:416:ILE:O	1:C:416:ILE:HG22	1.96	0.65
1:A:109:ARG:HA	1:A:112:ARG:NH2	2.12	0.65
1:A:172:TYR:OH	1:A:269:ASP:HA	1.96	0.65
1:B:244:ASP:HA	1:B:247:ASN:HD21	1.61	0.65
1:A:86:ASN:OD1	1:D:80:SER:HA	1.95	0.65
1:A:115:PHE:CD1	1:A:184:GLN:OE1	2.48	0.65
1:A:191:VAL:O	1:A:191:VAL:HG22	1.95	0.65
1:B:366:GLU:OE1	1:B:368:TYR:HE2	1.78	0.65
1:A:124:VAL:HG23	1:A:128:ARG:HG3	1.78	0.65
1:B:77:LYS:O	1:C:87:HIS:CD2	2.49	0.65
1:D:413:LEU:HA	1:D:416:ILE:HD11	1.78	0.65
1:B:172:TYR:OH	1:B:268:ARG:NH1	2.30	0.65
1:B:184:GLN:OE1	1:B:204:ARG:HD2	1.96	0.65
1:C:242:ASP:OD2	1:C:243:MET:HG3	1.97	0.65
1:C:265:LYS:HG2	1:C:268:ARG:HH22	1.62	0.64
1:C:45:ASP:OD1	1:C:46:PRO:N	2.30	0.64
1:D:265:LYS:HG2	1:D:268:ARG:HH21	1.61	0.64
1:A:88:LEU:HD13	1:D:74:ASP:HB3	1.79	0.64
1:A:65:VAL:HG23	1:D:90:HIS:CE1	2.32	0.64
1:A:254:ILE:O	1:A:254:ILE:HG23	1.97	0.64
1:A:71:LEU:CD1	1:A:107:VAL:HA	2.28	0.64
1:B:162:MET:HG2	1:B:188:MET:SD	2.37	0.64
1:C:267:LYS:HA	1:C:413:LEU:HD21	1.78	0.64
1:A:213:VAL:HA	1:A:287:ILE:O	1.97	0.64
1:B:151:ILE:HG13	1:B:202:VAL:HG13	1.80	0.64
1:C:273:LEU:HB2	1:C:278:ILE:HD12	1.80	0.64
1:D:410:LYS:HG2	1:D:410:LYS:O	1.97	0.64
1:C:70:MET:HE2	1:C:72:LEU:HG	1.80	0.64
1:D:257:GLU:O	1:D:261:ILE:CD1	2.45	0.64
1:A:211:LEU:HD13	1:A:367:VAL:HG11	1.79	0.64
1:C:216:LYS:HA	1:C:285:LEU:O	1.98	0.63
1:B:77:LYS:O	1:C:87:HIS:HD2	1.81	0.63
1:C:103:TYR:OH	1:C:190:ARG:HB2	1.98	0.63
1:C:266:LEU:O	1:C:270:VAL:HG23	1.99	0.63
1:A:279:MET:CE	1:A:279:MET:H	2.11	0.63
1:A:81:LYS:HB2	1:D:85:ASN:HD22	1.62	0.63
1:C:270:VAL:HB	1:C:413:LEU:HD21	1.79	0.63
1:D:183:PRO:HB2	1:D:185:PHE:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASP:O	1:A:195:ASN:ND2	2.32	0.63
1:B:261:ILE:O	1:B:264:GLU:HB2	1.99	0.63
1:B:54:GLY:HA3	1:B:100:PHE:CE1	2.34	0.63
1:A:62:LEU:HD12	1:D:89:PHE:CZ	2.33	0.63
1:D:120:GLN:OE1	1:D:120:GLN:HA	1.99	0.63
1:D:191:VAL:HG12	1:D:191:VAL:O	1.98	0.63
1:A:124:VAL:HG23	1:A:128:ARG:CG	2.29	0.63
1:B:163:HIS:CD2	1:B:188:MET:HE1	2.33	0.62
1:C:56:ALA:HA	1:C:123:LEU:HD13	1.80	0.62
1:B:206:MET:HE1	1:B:373:ILE:HG22	1.80	0.62
1:C:266:LEU:HD23	1:C:270:VAL:CG2	2.29	0.62
1:A:287:ILE:HG12	1:A:368:TYR:CD2	2.34	0.62
1:A:281:TYR:HA	1:A:374:ASP:HB3	1.79	0.62
1:B:273:LEU:O	1:B:278:ILE:HB	1.98	0.62
1:C:133:GLU:O	1:C:134:SER:CB	2.47	0.62
1:B:112:ARG:HG3	1:B:112:ARG:HH11	1.65	0.62
1:D:133:GLU:HA	1:D:142:LEU:CD2	2.29	0.62
1:A:117:ILE:HD11	1:A:204:ARG:HD2	1.81	0.62
1:B:185:PHE:CD1	1:B:201:LEU:HD21	2.33	0.62
1:C:270:VAL:CG2	1:C:413:LEU:HD21	2.30	0.62
1:B:45:ASP:OD1	1:B:48:VAL:HB	1.99	0.62
1:D:220:LYS:NZ	1:D:280:ASP:OD1	2.33	0.61
1:C:126:LEU:HD11	1:C:151:ILE:CD1	2.29	0.61
1:B:372:LEU:H	1:B:372:LEU:CD1	2.14	0.61
1:C:280:ASP:HA	1:C:408:TYR:CE2	2.35	0.61
1:A:261:ILE:O	1:A:264:GLU:HB2	2.01	0.61
1:D:261:ILE:O	1:D:264:GLU:HB2	2.01	0.61
1:B:159:ILE:HD12	1:B:188:MET:SD	2.39	0.61
1:C:70:MET:HE3	1:D:46:PRO:CG	2.27	0.61
1:A:120:GLN:O	1:A:124:VAL:HG12	2.01	0.61
1:B:180:THR:HB	1:B:269:ASP:OD1	2.00	0.61
1:D:132:SER:O	1:D:142:LEU:HD23	2.00	0.61
1:B:250:GLN:HG3	1:B:251:LYS:H	1.65	0.61
1:B:63:SER:OG	1:B:64:GLN:OE1	2.18	0.61
1:C:142:LEU:HD12	1:C:200:MET:HE3	1.82	0.61
1:B:90:HIS:CD2	1:C:65:VAL:HG22	2.36	0.61
1:A:195:ASN:O	1:A:195:ASN:OD1	2.19	0.60
1:C:207:PHE:HD1	1:C:369:PHE:HB2	1.66	0.60
1:A:413:LEU:HA	1:A:416:ILE:HD11	1.83	0.60
1:C:179:ASN:O	1:C:265:LYS:HD3	2.00	0.60
1:D:181:LEU:HB2	1:D:372:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:MET:HE1	1:D:46:PRO:HA	1.82	0.60
1:A:141:PHE:N	1:A:152:LYS:HA	2.15	0.60
1:B:270:VAL:HA	1:B:273:LEU:HD21	1.84	0.60
1:D:215:ARG:CG	1:D:215:ARG:NH1	2.59	0.60
1:B:108:PHE:HA	1:B:111:LEU:HB2	1.82	0.60
1:B:103:TYR:HB2	1:B:188:MET:O	2.02	0.60
1:B:206:MET:HE3	1:B:373:ILE:CG2	2.28	0.60
1:B:219:LEU:HD21	1:B:245:PHE:CD2	2.36	0.60
1:B:273:LEU:HD11	1:B:281:TYR:CE1	2.37	0.60
1:C:146:ASP:HB3	1:C:148:THR:OG1	2.02	0.60
1:C:131:PRO:HB3	1:C:144:SER:HA	1.82	0.60
1:C:154:VAL:O	1:C:199:TYR:HB2	2.01	0.60
1:C:102:GLU:HG3	1:C:189:TYR:CE2	2.37	0.60
1:A:47:LEU:HD11	1:A:198:SER:HB2	1.83	0.60
1:B:167:SER:O	1:B:170:HIS:HB3	2.02	0.60
1:C:270:VAL:HA	1:C:273:LEU:CD2	2.32	0.60
1:D:283:LEU:HD12	1:D:412:PHE:HZ	1.66	0.60
1:B:216:LYS:HB2	1:B:285:LEU:O	2.02	0.60
1:A:276:LEU:HB2	1:A:278:ILE:HG13	1.83	0.59
1:A:286:GLY:O	1:A:368:TYR:HA	2.01	0.59
1:A:266:LEU:HD21	1:A:412:PHE:CE2	2.36	0.59
1:C:201:LEU:HD23	1:C:202:VAL:N	2.17	0.59
1:A:286:GLY:N	1:A:369:PHE:O	2.35	0.59
1:B:112:ARG:HG3	1:B:112:ARG:NH1	2.18	0.59
1:B:193:VAL:O	1:B:196:GLU:HG3	2.01	0.59
1:C:270:VAL:HG21	1:C:413:LEU:CG	2.32	0.59
1:D:104:CYS:CB	1:D:107:VAL:HB	2.32	0.59
1:D:176:CYS:SG	1:D:180:THR:HG22	2.42	0.59
1:D:274:VAL:HG12	1:D:275:GLN:N	2.16	0.59
1:A:410:LYS:HG2	1:A:410:LYS:O	2.01	0.59
1:C:287:ILE:HG21	1:C:366:GLU:OE2	2.03	0.59
1:B:82:ILE:HD12	1:C:84:VAL:HG22	1.84	0.59
1:A:103:TYR:HB2	1:A:188:MET:CG	2.26	0.59
1:C:207:PHE:CD1	1:C:213:VAL:HG21	2.38	0.59
1:C:72:LEU:O	1:C:75:ASP:HB2	2.02	0.59
1:B:260:LYS:O	1:B:263:LEU:HB2	2.02	0.59
1:B:285:LEU:HD22	1:B:286:GLY:N	2.13	0.59
1:B:50:VAL:HG21	1:B:98:PHE:HB2	1.85	0.59
1:C:210:ARG:O	1:C:212:PRO:HD3	2.03	0.59
1:A:59:ILE:HD13	1:A:123:LEU:CB	2.33	0.59
1:B:87:HIS:O	1:B:88:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:GLU:HG2	1:C:134:SER:H	1.68	0.59
1:B:103:TYR:CB	1:B:188:MET:HG2	2.32	0.59
1:A:155:SER:O	1:A:158:ASP:HB2	2.03	0.58
1:A:182:LEU:HD22	1:A:375:ILE:HG21	1.84	0.58
1:B:59:ILE:HG13	1:B:123:LEU:CD1	2.32	0.58
1:D:62:LEU:O	1:D:109:ARG:NH2	2.36	0.58
1:D:47:LEU:HD11	1:D:200:MET:HE1	1.84	0.58
1:B:51:PHE:HE2	1:B:151:ILE:HD13	1.68	0.58
1:B:273:LEU:HD23	1:B:273:LEU:H	1.68	0.58
1:A:266:LEU:HD23	1:A:413:LEU:CD2	2.33	0.58
1:B:143:ILE:HG23	1:B:147:ARG:HA	1.83	0.58
1:B:281:TYR:HB3	1:B:375:ILE:HG22	1.85	0.58
1:C:287:ILE:HG23	1:C:366:GLU:HB3	1.85	0.58
1:C:46:PRO:O	1:C:193:VAL:HG21	2.03	0.58
1:A:87:HIS:O	1:A:88:LEU:HB2	2.02	0.58
1:B:99:LYS:HB2	1:B:192:SER:CB	2.33	0.58
1:C:270:VAL:HG21	1:C:413:LEU:CD2	2.34	0.58
1:D:288:HIS:HB3	1:D:367:VAL:HB	1.85	0.58
1:A:146:ASP:HB3	1:A:148:THR:OG1	2.04	0.58
1:A:156:SER:HB2	1:A:199:TYR:CZ	2.38	0.58
1:A:375:ILE:HG13	1:A:376:LEU:HD12	1.85	0.58
1:B:206:MET:CE	1:B:373:ILE:CG2	2.74	0.58
1:D:115:PHE:HZ	1:D:169:TYR:HH	1.52	0.58
1:A:115:PHE:CZ	1:A:184:GLN:HG2	2.38	0.58
1:B:143:ILE:CG2	1:B:147:ARG:HA	2.34	0.58
1:A:274:VAL:HG13	1:A:405:PRO:CB	2.33	0.57
1:A:417:THR:HG23	1:A:417:THR:O	2.00	0.57
1:C:124:VAL:HG23	1:C:128:ARG:HB2	1.86	0.57
1:C:103:TYR:CD1	1:C:188:MET:HG2	2.39	0.57
1:D:276:LEU:HB2	1:D:278:ILE:HG13	1.85	0.57
1:A:76:PHE:CD2	1:A:166:LEU:HD23	2.39	0.57
1:B:102:GLU:OE2	1:B:105:PRO:HA	2.04	0.57
1:B:56:ALA:HA	1:B:123:LEU:HD11	1.86	0.57
1:B:263:LEU:O	1:B:264:GLU:C	2.42	0.57
1:C:265:LYS:HA	1:C:268:ARG:NH1	2.18	0.57
1:C:268:ARG:HG3	1:C:269:ASP:N	2.19	0.57
1:B:265:LYS:CG	1:B:268:ARG:HH21	2.17	0.57
1:B:270:VAL:HG11	1:B:413:LEU:HD11	1.86	0.57
1:B:74:ASP:HB3	1:C:88:LEU:HD13	1.87	0.57
1:C:169:TYR:CE2	1:C:173:ILE:HD11	2.40	0.57
1:B:59:ILE:HG21	1:B:123:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASP:O	1:C:125:SER:HB2	2.04	0.57
1:C:266:LEU:HD23	1:C:270:VAL:HG21	1.86	0.57
1:A:154:VAL:HB	1:A:158:ASP:CB	2.35	0.57
1:A:366:GLU:HB3	1:A:368:TYR:CE1	2.33	0.57
1:B:76:PHE:CE2	1:B:167:SER:HA	2.39	0.57
1:B:120:GLN:O	1:B:124:VAL:HG12	2.05	0.57
1:A:217:TYR:CD1	1:A:285:LEU:HD12	2.40	0.57
1:D:212:PRO:HD2	1:D:288:HIS:ND1	2.20	0.57
1:A:52:LEU:CD2	1:A:127:THR:HA	2.35	0.57
1:B:412:PHE:CE2	1:B:416:ILE:CD1	2.88	0.57
1:C:169:TYR:CZ	1:C:173:ILE:HD11	2.40	0.57
1:D:111:LEU:HD23	1:D:173:ILE:HG21	1.85	0.57
1:A:165:ASN:O	1:A:169:TYR:HB2	2.05	0.56
1:B:103:TYR:CG	1:B:188:MET:HG2	2.39	0.56
1:B:146:ASP:O	1:B:148:THR:HG23	2.04	0.56
1:B:54:GLY:HA3	1:B:100:PHE:CZ	2.40	0.56
1:D:181:LEU:HB2	1:D:372:LEU:CD1	2.34	0.56
1:D:47:LEU:HD12	1:D:191:VAL:CG1	2.35	0.56
1:B:59:ILE:HG13	1:B:123:LEU:HD12	1.87	0.56
1:A:169:TYR:O	1:A:173:ILE:HG12	2.04	0.56
1:B:81:LYS:HA	1:B:100:PHE:O	2.05	0.56
1:B:146:ASP:HB3	1:B:148:THR:OG1	2.05	0.56
1:A:70:MET:CE	1:B:46:PRO:HA	2.35	0.56
1:C:70:MET:CE	1:C:72:LEU:HG	2.36	0.56
1:D:169:TYR:CE1	1:D:173:ILE:HD11	2.41	0.56
1:D:271:GLU:O	1:D:274:VAL:HB	2.05	0.56
1:A:268:ARG:HG3	1:A:269:ASP:N	2.20	0.56
1:B:172:TYR:OH	1:B:269:ASP:OD1	2.20	0.56
1:B:71:LEU:HD22	1:B:75:ASP:OD2	2.06	0.56
1:B:90:HIS:ND1	1:B:92:GLU:N	2.48	0.56
1:A:217:TYR:HB2	1:A:285:LEU:CB	2.35	0.56
1:A:217:TYR:HB3	1:A:219:LEU:CD2	2.35	0.56
1:C:215:ARG:O	1:C:286:GLY:HA2	2.05	0.56
1:D:83:LYS:HD2	1:D:99:LYS:CE	2.35	0.56
1:A:276:LEU:HB2	1:A:278:ILE:CG1	2.35	0.56
1:B:56:ALA:HA	1:B:123:LEU:CD1	2.36	0.56
1:C:50:VAL:CG1	1:C:191:VAL:HG23	2.36	0.56
1:A:268:ARG:O	1:A:271:GLU:HB3	2.06	0.56
1:C:50:VAL:HG11	1:C:191:VAL:HG23	1.87	0.56
1:C:242:ASP:OD1	1:C:415:PHE:CZ	2.58	0.56
1:A:59:ILE:CG2	1:A:123:LEU:HD22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HG23	1:B:178:GLY:CA	2.35	0.56
1:D:161:ASP:HA	1:D:164:SER:OG	2.06	0.56
1:B:50:VAL:HG22	1:B:98:PHE:CD2	2.41	0.56
1:A:216:LYS:HA	1:A:285:LEU:O	2.06	0.55
1:A:49:GLY:HA2	1:A:52:LEU:CD1	2.35	0.55
1:A:54:GLY:HA3	1:A:100:PHE:CE1	2.40	0.55
1:C:45:ASP:OD1	1:C:46:PRO:CD	2.54	0.55
1:D:209:HIS:CD2	1:D:209:HIS:H	2.24	0.55
1:A:47:LEU:HD12	1:A:191:VAL:CG2	2.27	0.55
1:D:81:LYS:HA	1:D:100:PHE:O	2.07	0.55
1:D:375:ILE:O	1:D:376:LEU:HD23	2.05	0.55
1:A:83:LYS:CD	1:A:99:LYS:HD3	2.15	0.55
1:B:102:GLU:OE1	1:B:105:PRO:HG3	2.07	0.55
1:B:141:PHE:CD1	1:B:152:LYS:HB2	2.41	0.55
1:B:366:GLU:O	1:B:368:TYR:CZ	2.59	0.55
1:C:123:LEU:HD12	1:C:127:THR:OG1	2.06	0.55
1:A:90:HIS:CD2	1:A:92:GLU:N	2.73	0.55
1:B:117:ILE:CD1	1:B:186:LEU:HD22	2.37	0.55
1:C:115:PHE:CD2	1:C:184:GLN:HB3	2.41	0.55
1:D:259:LYS:C	1:D:263:LEU:HD12	2.26	0.55
1:D:81:LYS:CD	1:D:101:LYS:HE3	2.35	0.55
1:B:189:TYR:CD1	1:B:189:TYR:N	2.74	0.55
1:B:271:GLU:HA	1:B:274:VAL:HB	1.89	0.55
1:B:106:GLN:OE1	1:B:106:GLN:HA	2.06	0.55
1:D:276:LEU:O	1:D:277:LYS:HB2	2.07	0.55
1:C:208:SER:HB3	1:C:211:LEU:O	2.07	0.54
1:A:88:LEU:HD13	1:D:74:ASP:CB	2.37	0.54
1:A:117:ILE:HD12	1:A:186:LEU:CD2	2.37	0.54
1:A:71:LEU:HD11	1:A:107:VAL:HA	1.89	0.54
1:C:104:CYS:HB3	1:C:107:VAL:CG2	2.38	0.54
1:C:70:MET:HE1	1:D:46:PRO:CA	2.37	0.54
1:D:115:PHE:HB3	1:D:117:ILE:HD12	1.88	0.54
1:D:245:PHE:CD1	1:D:250:GLN:HB2	2.42	0.54
1:D:51:PHE:CE2	1:D:151:ILE:HD13	2.41	0.54
1:C:267:LYS:O	1:C:271:GLU:OE1	2.25	0.54
1:B:281:TYR:CB	1:B:375:ILE:HG22	2.38	0.54
1:D:188:MET:HG3	1:D:201:LEU:CD1	2.37	0.54
1:B:122:TYR:CE1	1:B:149:LEU:HD13	2.42	0.54
1:C:103:TYR:CD1	1:C:188:MET:O	2.54	0.54
1:C:259:LYS:O	1:C:263:LEU:HG	2.07	0.54
1:D:183:PRO:HB2	1:D:185:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LYS:C	1:A:263:LEU:HD12	2.28	0.54
1:B:147:ARG:HH11	1:B:147:ARG:HG2	1.72	0.54
1:A:70:MET:HE3	1:B:46:PRO:HA	1.88	0.54
1:D:149:LEU:HD22	1:D:204:ARG:HA	1.89	0.54
1:A:114:ARG:CZ	1:A:174:VAL:HG13	2.38	0.54
1:D:187:GLY:HA3	1:D:202:VAL:HB	1.89	0.54
1:A:70:MET:HG2	1:A:70:MET:O	2.07	0.54
1:A:78:ALA:HB2	1:D:88:LEU:HB2	1.90	0.54
1:A:151:ILE:CG2	1:A:202:VAL:HG22	2.38	0.54
1:D:287:ILE:HA	1:D:367:VAL:O	2.07	0.54
1:A:52:LEU:HD23	1:A:127:THR:HA	1.90	0.53
1:C:216:LYS:O	1:C:216:LYS:HG2	2.08	0.53
1:B:216:LYS:HA	1:B:285:LEU:O	2.07	0.53
1:B:82:ILE:CD1	1:C:84:VAL:HG22	2.38	0.53
1:A:284:LEU:O	1:A:370:MET:HA	2.08	0.53
1:B:89:PHE:HE1	1:C:106:GLN:HG2	1.71	0.53
1:B:90:HIS:CE1	1:B:92:GLU:N	2.66	0.53
1:C:412:PHE:CE1	1:C:416:ILE:CD1	2.91	0.53
1:D:143:ILE:CG2	1:D:147:ARG:HA	2.36	0.53
1:A:272:PHE:HA	1:A:275:GLN:CD	2.28	0.53
1:C:45:ASP:OD1	1:C:46:PRO:HD2	2.08	0.53
1:D:104:CYS:HB3	1:D:107:VAL:CG2	2.39	0.53
1:A:74:ASP:HA	1:A:77:LYS:CG	2.38	0.53
1:B:176:CYS:O	1:B:179:ASN:OD1	2.26	0.53
1:B:185:PHE:CE1	1:B:201:LEU:HD21	2.43	0.53
1:B:273:LEU:HB2	1:B:278:ILE:CB	2.39	0.53
1:A:59:ILE:HD11	1:A:122:TYR:CD2	2.44	0.53
1:A:215:ARG:HB2	1:A:287:ILE:HB	1.90	0.53
1:B:74:ASP:HA	1:B:77:LYS:HG3	1.90	0.53
1:C:195:ASN:OD1	1:C:195:ASN:O	2.27	0.53
1:B:240:LEU:HB3	1:B:244:ASP:HB2	1.89	0.53
1:B:273:LEU:HD23	1:B:273:LEU:N	2.24	0.53
1:C:270:VAL:CB	1:C:413:LEU:HD21	2.39	0.53
1:D:50:VAL:HA	1:D:94:LEU:HD22	1.88	0.53
1:C:172:TYR:CE2	1:C:176:CYS:HB2	2.43	0.53
1:D:242:ASP:HB2	1:D:415:PHE:HZ	1.74	0.53
1:D:182:LEU:HD11	1:D:272:PHE:CD2	2.43	0.53
1:A:74:ASP:O	1:D:88:LEU:HD13	2.08	0.53
1:A:117:ILE:HD12	1:A:186:LEU:HD21	1.89	0.53
1:D:220:LYS:NZ	1:D:280:ASP:OD2	2.42	0.53
1:B:417:THR:CG2	1:B:417:THR:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:PHE:CG	1:C:184:GLN:HB3	2.44	0.53
1:D:104:CYS:HB2	1:D:107:VAL:HB	1.90	0.53
1:D:115:PHE:CE1	1:D:184:GLN:HG2	2.44	0.52
1:A:52:LEU:CB	1:A:127:THR:HG22	2.34	0.52
1:A:281:TYR:HA	1:A:374:ASP:O	2.09	0.52
1:B:54:GLY:HA3	1:B:100:PHE:CD1	2.43	0.52
1:B:147:ARG:NH1	1:B:147:ARG:HG2	2.23	0.52
1:C:51:PHE:CE2	1:C:151:ILE:HD13	2.43	0.52
1:C:70:MET:CE	1:D:46:PRO:CG	2.84	0.52
1:A:126:LEU:CD1	1:A:202:VAL:HG11	2.36	0.52
1:A:72:LEU:HD11	1:B:95:PRO:CG	2.37	0.52
1:B:273:LEU:HD12	1:B:278:ILE:CG2	2.38	0.52
1:B:220:LYS:HG3	1:B:282:SER:OG	2.08	0.52
1:C:273:LEU:CA	1:C:278:ILE:HD12	2.37	0.52
1:A:273:LEU:O	1:A:273:LEU:HD23	2.09	0.52
1:A:57:HIS:O	1:A:61:GLU:HB2	2.09	0.52
1:B:169:TYR:CZ	1:B:185:PHE:HD2	2.28	0.52
1:B:287:ILE:HA	1:B:367:VAL:O	2.10	0.52
1:C:84:VAL:O	1:C:97:HIS:HA	2.10	0.52
1:A:106:GLN:HA	1:A:106:GLN:OE1	2.10	0.52
1:B:103:TYR:HB3	1:B:188:MET:HE2	1.91	0.52
1:D:65:VAL:HG12	1:D:109:ARG:CZ	2.39	0.52
1:D:195:ASN:OD1	1:D:195:ASN:O	2.28	0.52
1:D:262:PHE:CE2	1:D:266:LEU:HD12	2.44	0.52
1:C:47:LEU:HG	1:C:48:VAL:N	2.23	0.52
1:D:150:VAL:HG23	1:D:205:ASN:HB2	1.90	0.52
1:A:72:LEU:HD21	1:B:95:PRO:HA	0.73	0.52
1:C:92:GLU:HG3	1:C:92:GLU:O	2.10	0.52
1:D:135:GLU:HA	1:D:135:GLU:OE1	2.09	0.52
1:D:170:HIS:NE2	1:D:174:VAL:HG22	2.25	0.52
1:D:242:ASP:HB2	1:D:415:PHE:CZ	2.45	0.52
1:C:143:ILE:CG2	1:C:147:ARG:HA	2.40	0.52
1:C:266:LEU:HD21	1:C:412:PHE:CE2	2.45	0.52
1:A:107:VAL:HG11	1:A:166:LEU:CD2	2.40	0.51
1:B:218:ASP:HB2	1:B:239:THR:CG2	2.40	0.51
1:B:71:LEU:HD12	1:B:170:HIS:CE1	2.44	0.51
1:C:142:LEU:HD12	1:C:200:MET:CE	2.40	0.51
1:C:267:LYS:CA	1:C:413:LEU:HD22	2.36	0.51
1:D:180:THR:HG1	1:D:182:LEU:H	1.58	0.51
1:C:70:MET:CE	1:D:93:ASN:O	2.57	0.51
1:A:162:MET:HE1	1:A:185:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:HIS:H	1:A:209:HIS:CD2	2.26	0.51
1:A:217:TYR:N	1:A:285:LEU:HB3	2.20	0.51
1:C:83:LYS:CG	1:C:99:LYS:HE3	2.41	0.51
1:D:104:CYS:HB3	1:D:107:VAL:HB	1.91	0.51
1:A:54:GLY:HA3	1:A:100:PHE:CD1	2.46	0.51
1:A:59:ILE:HD13	1:A:123:LEU:HA	1.92	0.51
1:B:283:LEU:HD13	1:B:416:ILE:HD12	1.91	0.51
1:A:173:ILE:HG23	1:A:178:GLY:CA	2.40	0.51
1:B:149:LEU:HD22	1:B:186:LEU:CD1	2.40	0.51
1:C:285:LEU:HD12	1:C:370:MET:CG	2.38	0.51
1:C:267:LYS:CA	1:C:413:LEU:CD2	2.86	0.51
1:D:268:ARG:HG3	1:D:269:ASP:N	2.26	0.51
1:D:270:VAL:HG13	1:D:281:TYR:OH	2.10	0.51
1:A:274:VAL:CG1	1:A:405:PRO:HB3	2.36	0.51
1:B:220:LYS:HE3	1:B:282:SER:OG	2.11	0.51
1:B:54:GLY:O	1:B:57:HIS:HB3	2.11	0.51
1:C:104:CYS:SG	1:C:163:HIS:CE1	3.04	0.51
1:D:283:LEU:HD13	1:D:412:PHE:HZ	1.73	0.51
1:A:133:GLU:HG3	1:A:142:LEU:HD23	1.93	0.51
1:C:414:ASP:O	1:C:417:THR:HG22	2.09	0.51
1:A:220:LYS:NZ	1:A:220:LYS:HB2	2.26	0.51
1:C:159:ILE:HD12	1:C:188:MET:SD	2.51	0.51
1:D:83:LYS:HD2	1:D:99:LYS:HE3	1.92	0.51
1:C:79:SER:HB2	1:C:101:LYS:HE2	1.92	0.51
1:D:283:LEU:HD12	1:D:372:LEU:HG	1.93	0.51
1:A:51:PHE:CE2	1:A:126:LEU:HD21	2.46	0.51
1:B:287:ILE:HG23	1:B:366:GLU:HB2	1.92	0.51
1:D:150:VAL:HG23	1:D:205:ASN:CB	2.41	0.51
1:D:193:VAL:HG12	1:D:193:VAL:O	2.10	0.51
1:D:273:LEU:HA	1:D:278:ILE:HD12	1.93	0.51
1:A:146:ASP:OD1	1:A:148:THR:HG23	2.11	0.51
1:A:273:LEU:O	1:A:278:ILE:HB	2.11	0.51
1:C:215:ARG:HG2	1:C:215:ARG:HH11	1.76	0.51
1:C:83:LYS:HD2	1:C:99:LYS:HZ2	1.73	0.51
1:D:408:TYR:O	1:D:411:ARG:HB2	2.11	0.51
1:C:161:ASP:HA	1:C:164:SER:OG	2.11	0.50
1:A:74:ASP:CA	1:A:77:LYS:HE3	2.35	0.50
1:C:121:ASP:HA	1:C:124:VAL:HG12	1.93	0.50
1:C:162:MET:HG3	1:C:188:MET:SD	2.51	0.50
1:A:411:ARG:O	1:A:415:PHE:HB2	2.11	0.50
1:B:274:VAL:HG12	1:B:275:GLN:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:TYR:OH	1:C:202:VAL:HG21	2.11	0.50
1:D:262:PHE:CZ	1:D:266:LEU:HD12	2.45	0.50
1:A:93:ASN:OD1	1:A:94:LEU:HG	2.10	0.50
1:C:268:ARG:HH11	1:C:268:ARG:HG2	1.75	0.50
1:C:416:ILE:O	1:C:416:ILE:CG2	2.59	0.50
1:A:78:ALA:CB	1:D:88:LEU:HB2	2.41	0.50
1:C:149:LEU:HD13	1:C:186:LEU:HD12	1.94	0.50
1:D:417:THR:O	1:D:417:THR:CG2	2.56	0.50
1:B:217:TYR:CD2	1:B:240:LEU:HD12	2.46	0.50
1:B:273:LEU:HD11	1:B:281:TYR:CD1	2.46	0.50
1:C:192:SER:HB3	1:C:197:ASP:OD1	2.11	0.50
1:A:80:SER:OG	1:A:80:SER:O	2.26	0.50
1:B:71:LEU:HD11	1:B:107:VAL:HA	1.93	0.50
1:A:132:SER:O	1:A:143:ILE:N	2.45	0.50
1:A:176:CYS:SG	1:A:180:THR:HG22	2.52	0.50
1:A:288:HIS:HB3	1:A:367:VAL:CB	2.37	0.50
1:B:176:CYS:SG	1:B:180:THR:HG22	2.51	0.50
1:C:172:TYR:OH	1:C:268:ARG:NE	2.45	0.50
1:C:58:SER:O	1:C:62:LEU:HB2	2.12	0.50
1:A:146:ASP:O	1:A:146:ASP:OD1	2.29	0.50
1:A:76:PHE:CE2	1:A:167:SER:HA	2.46	0.50
1:D:124:VAL:CG1	1:D:125:SER:N	2.75	0.50
1:D:121:ASP:HA	1:D:124:VAL:HG12	1.92	0.50
1:C:90:HIS:O	1:C:91:ARG:HB2	2.12	0.49
1:D:56:ALA:O	1:D:60:ASN:OD1	2.30	0.49
1:A:65:VAL:HG21	1:D:90:HIS:HA	1.92	0.49
1:B:141:PHE:HE1	1:B:152:LYS:HB2	1.73	0.49
1:D:87:HIS:CD2	1:D:88:LEU:HG	2.47	0.49
1:A:124:VAL:HG23	1:A:128:ARG:CD	2.43	0.49
1:B:266:LEU:HD11	1:B:416:ILE:CG1	2.38	0.49
1:B:70:MET:HE2	1:B:72:LEU:HG	1.93	0.49
1:C:278:ILE:HG21	1:C:375:ILE:HG23	1.94	0.49
1:D:266:LEU:HD11	1:D:416:ILE:HD12	1.94	0.49
1:A:112:ARG:HH11	1:A:112:ARG:HG3	1.77	0.49
1:A:57:HIS:CE1	1:A:82:ILE:HG13	2.46	0.49
1:B:219:LEU:HD21	1:B:245:PHE:CE2	2.47	0.49
1:C:273:LEU:O	1:C:278:ILE:HB	2.12	0.49
1:B:90:HIS:CD2	1:C:65:VAL:CG2	2.95	0.49
1:D:124:VAL:O	1:D:128:ARG:HB2	2.12	0.49
1:D:180:THR:HG1	1:D:182:LEU:HB2	1.76	0.49
1:C:107:VAL:O	1:C:110:ASN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:CG2	1:C:128:ARG:HD3	2.40	0.49
1:D:168:ASN:O	1:D:171:GLN:HB2	2.12	0.49
1:A:126:LEU:HD23	1:A:126:LEU:O	2.12	0.49
1:A:217:TYR:HB2	1:A:285:LEU:HB3	1.94	0.49
1:C:270:VAL:HA	1:C:273:LEU:HD23	1.94	0.49
1:C:72:LEU:HD23	1:D:95:PRO:HA	1.94	0.49
1:A:117:ILE:CG2	1:A:122:TYR:HB2	2.43	0.49
1:B:273:LEU:CD2	1:B:273:LEU:H	2.25	0.49
1:C:133:GLU:O	1:C:134:SER:HB2	2.12	0.49
1:A:266:LEU:CD2	1:A:416:ILE:HD11	2.43	0.49
1:B:62:LEU:O	1:B:109:ARG:NH2	2.46	0.49
1:B:74:ASP:HA	1:B:77:LYS:CG	2.43	0.49
1:C:162:MET:HB3	1:C:188:MET:HE1	1.94	0.49
1:D:65:VAL:HG12	1:D:109:ARG:NH1	2.27	0.49
1:D:148:THR:O	1:D:149:LEU:HD23	2.13	0.49
1:D:281:TYR:O	1:D:408:TYR:OH	2.29	0.49
1:A:277:LYS:HG2	1:A:277:LYS:O	2.13	0.49
1:D:207:PHE:HE2	1:D:216:LYS:HE3	1.78	0.49
1:A:285:LEU:HD22	1:A:286:GLY:H	1.77	0.49
1:C:90:HIS:O	1:C:91:ARG:CB	2.60	0.49
1:D:62:LEU:O	1:D:65:VAL:HB	2.13	0.49
1:A:133:GLU:CG	1:A:142:LEU:HD23	2.43	0.48
1:A:51:PHE:CE2	1:A:151:ILE:HD13	2.42	0.48
1:B:265:LYS:HG2	1:B:268:ARG:NH2	2.26	0.48
1:A:50:VAL:HG21	1:A:193:VAL:CG2	2.43	0.48
1:A:278:ILE:HA	1:A:279:MET:CE	2.43	0.48
1:A:408:TYR:O	1:A:408:TYR:CG	2.66	0.48
1:B:412:PHE:O	1:B:415:PHE:HB3	2.12	0.48
1:C:106:GLN:OE1	1:C:109:ARG:NH1	2.45	0.48
1:C:153:GLU:HG3	1:C:154:VAL:N	2.28	0.48
1:D:266:LEU:HD21	1:D:412:PHE:CE2	2.48	0.48
1:C:266:LEU:CD2	1:C:270:VAL:HG21	2.42	0.48
1:D:47:LEU:HD11	1:D:198:SER:HB2	1.95	0.48
1:A:80:SER:HB2	1:D:86:ASN:OD1	2.14	0.48
1:B:147:ARG:HB3	1:B:209:HIS:HA	1.94	0.48
1:B:289:ASP:OD2	1:B:290:ILE:N	2.46	0.48
1:D:285:LEU:HD22	1:D:286:GLY:N	2.29	0.48
1:A:85:ASN:OD1	1:A:97:HIS:ND1	2.47	0.48
1:A:155:SER:HB3	1:A:158:ASP:OD1	2.14	0.48
1:C:124:VAL:HG21	1:C:128:ARG:NH1	2.29	0.48
1:C:92:GLU:O	1:C:93:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASP:CA	1:D:77:LYS:HG3	2.40	0.48
1:D:121:ASP:N	1:D:121:ASP:OD1	2.45	0.48
1:D:207:PHE:CZ	1:D:284:LEU:HD11	2.49	0.48
1:A:180:THR:HB	1:A:269:ASP:CG	2.34	0.48
1:B:51:PHE:CE2	1:B:151:ILE:HG21	2.49	0.48
1:C:273:LEU:CB	1:C:278:ILE:HD12	2.42	0.48
1:C:45:ASP:O	1:C:49:GLY:HA3	2.13	0.48
1:A:170:HIS:O	1:A:174:VAL:HG23	2.14	0.48
1:A:373:ILE:CG1	1:A:374:ASP:N	2.74	0.48
1:B:176:CYS:O	1:B:177:HIS:HB2	2.14	0.48
1:B:239:THR:O	1:B:239:THR:HG22	2.14	0.48
1:C:126:LEU:CD1	1:C:151:ILE:HD11	2.42	0.48
1:C:201:LEU:HD22	1:C:203:MET:HG2	1.95	0.48
1:A:411:ARG:O	1:A:415:PHE:CB	2.62	0.47
1:B:94:LEU:HD12	1:B:98:PHE:CZ	2.49	0.47
1:C:115:PHE:CE2	1:C:184:GLN:HB3	2.49	0.47
1:C:151:ILE:HA	1:C:201:LEU:O	2.14	0.47
1:B:244:ASP:O	1:B:248:LYS:HG2	2.14	0.47
1:B:215:ARG:HB3	1:B:287:ILE:HD12	1.96	0.47
1:C:182:LEU:HD23	1:C:375:ILE:HD11	1.95	0.47
1:D:190:ARG:HB2	1:D:199:TYR:CD2	2.49	0.47
1:A:59:ILE:HD13	1:A:123:LEU:CA	2.44	0.47
1:A:159:ILE:O	1:A:162:MET:HB2	2.13	0.47
1:B:412:PHE:CE2	1:B:416:ILE:HD13	2.44	0.47
1:C:260:LYS:HA	1:C:263:LEU:HD12	1.95	0.47
1:D:119:ASP:HA	1:D:122:TYR:HB3	1.95	0.47
1:D:79:SER:OG	1:D:101:LYS:HE2	2.15	0.47
1:D:115:PHE:HZ	1:D:169:TYR:OH	1.97	0.47
1:D:164:SER:HG	1:D:165:ASN:H	1.61	0.47
1:A:59:ILE:HG21	1:A:123:LEU:HD22	1.95	0.47
1:A:65:VAL:HG12	1:A:65:VAL:O	2.15	0.47
1:C:207:PHE:CD1	1:C:369:PHE:HB2	2.47	0.47
1:C:266:LEU:HD23	1:C:270:VAL:HG23	1.96	0.47
1:C:373:ILE:C	1:C:373:ILE:HD13	2.35	0.47
1:D:47:LEU:HD11	1:D:200:MET:CE	2.45	0.47
1:D:216:LYS:O	1:D:216:LYS:HG2	2.14	0.47
1:C:273:LEU:HG	1:C:274:VAL:N	2.29	0.47
1:D:283:LEU:HD13	1:D:412:PHE:CZ	2.49	0.47
1:A:159:ILE:HG22	1:A:160:ALA:N	2.29	0.47
1:B:93:ASN:O	1:B:93:ASN:OD1	2.32	0.47
1:D:176:CYS:O	1:D:179:ASN:OD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ARG:HG3	1:D:211:LEU:N	2.29	0.47
1:B:167:SER:O	1:B:170:HIS:N	2.47	0.47
1:B:167:SER:O	1:B:171:GLN:HG2	2.14	0.47
1:B:266:LEU:CD2	1:B:416:ILE:HD11	2.24	0.47
1:C:51:PHE:HE2	1:C:151:ILE:HD13	1.80	0.47
1:D:215:ARG:HB2	1:D:287:ILE:HB	1.95	0.47
1:D:83:LYS:HD2	1:D:99:LYS:HE2	1.96	0.47
1:A:110:ASN:OD1	1:A:170:HIS:NE2	2.47	0.47
1:A:117:ILE:HG22	1:A:122:TYR:HB2	1.97	0.47
1:B:273:LEU:HB2	1:B:278:ILE:CD1	2.44	0.47
1:C:104:CYS:HB3	1:C:107:VAL:HG21	1.95	0.47
1:A:81:LYS:CB	1:D:85:ASN:HD22	2.28	0.47
1:A:283:LEU:HB2	1:A:412:PHE:CZ	2.49	0.47
1:C:140:ARG:O	1:C:141:PHE:C	2.53	0.47
1:A:117:ILE:HD13	1:A:186:LEU:HD13	1.97	0.47
1:A:118:ASP:O	1:A:121:ASP:N	2.48	0.47
1:A:171:GLN:HA	1:A:174:VAL:HG23	1.97	0.47
1:A:408:TYR:O	1:A:408:TYR:CD1	2.68	0.47
1:D:184:GLN:O	1:D:203:MET:HB3	2.14	0.47
1:B:54:GLY:HA3	1:B:100:PHE:CE2	2.51	0.46
1:A:154:VAL:HB	1:A:158:ASP:HB2	1.95	0.46
1:A:273:LEU:HD11	1:A:375:ILE:HB	1.97	0.46
1:B:47:LEU:HG	1:B:191:VAL:CG2	2.45	0.46
1:B:98:PHE:CB	1:B:193:VAL:HG22	2.45	0.46
1:C:252:VAL:HG12	1:C:252:VAL:O	2.13	0.46
1:D:140:ARG:HB2	1:D:153:GLU:HB2	1.97	0.46
1:D:160:ALA:O	1:D:164:SER:N	2.47	0.46
1:A:62:LEU:HD11	1:A:105:PRO:HB3	1.97	0.46
1:B:218:ASP:HB2	1:B:239:THR:HG22	1.97	0.46
1:B:260:LYS:HE2	1:B:260:LYS:HB2	1.51	0.46
1:B:371:GLY:O	1:B:373:ILE:HG23	2.14	0.46
1:C:62:LEU:O	1:C:109:ARG:NH2	2.48	0.46
1:D:159:ILE:O	1:D:162:MET:HB3	2.15	0.46
1:A:153:GLU:HG3	1:A:154:VAL:N	2.29	0.46
1:A:281:TYR:CD1	1:A:372:LEU:CD1	2.94	0.46
1:B:59:ILE:CG2	1:B:123:LEU:HD13	2.45	0.46
1:B:273:LEU:HD13	1:B:375:ILE:HG21	1.96	0.46
1:C:87:HIS:CE1	1:C:88:LEU:HG	2.51	0.46
1:D:163:HIS:O	1:D:166:LEU:HB3	2.16	0.46
1:A:191:VAL:CG2	1:A:191:VAL:O	2.61	0.46
1:C:266:LEU:CD2	1:C:270:VAL:CG2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:VAL:HA	1:D:287:ILE:O	2.16	0.46
1:B:273:LEU:HB2	1:B:278:ILE:CG1	2.46	0.46
1:A:62:LEU:O	1:A:109:ARG:NH2	2.49	0.46
1:A:151:ILE:HG23	1:A:202:VAL:HG13	1.98	0.46
1:C:207:PHE:CE1	1:C:213:VAL:HG21	2.51	0.46
1:C:181:LEU:HD12	1:C:266:LEU:HA	1.98	0.46
1:D:103:TYR:HB3	1:D:163:HIS:NE2	2.31	0.46
1:D:143:ILE:HG22	1:D:144:SER:O	2.16	0.46
1:D:90:HIS:HB3	1:D:91:ARG:H	1.49	0.46
1:A:118:ASP:O	1:A:121:ASP:HB2	2.16	0.46
1:B:265:LYS:O	1:B:266:LEU:C	2.53	0.46
1:B:217:TYR:CE1	1:B:285:LEU:HD12	2.51	0.46
1:C:255:GLY:HA3	1:C:258:GLU:CD	2.35	0.46
1:D:149:LEU:CD2	1:D:204:ARG:HA	2.45	0.46
1:A:212:PRO:HD2	1:A:288:HIS:CD2	2.50	0.46
1:B:277:LYS:HD3	1:B:277:LYS:O	2.15	0.46
1:B:99:LYS:N	1:B:192:SER:O	2.49	0.46
1:C:373:ILE:O	1:C:373:ILE:HG12	2.16	0.46
1:C:50:VAL:O	1:C:54:GLY:N	2.47	0.46
1:C:83:LYS:HD2	1:C:99:LYS:HZ1	1.76	0.46
1:D:160:ALA:O	1:D:163:HIS:N	2.49	0.46
1:A:47:LEU:CD1	1:A:191:VAL:O	2.64	0.45
1:A:266:LEU:HD21	1:A:416:ILE:HD11	1.99	0.45
1:C:101:LYS:HB2	1:C:190:ARG:NH2	2.31	0.45
1:C:157:GLU:O	1:C:160:ALA:N	2.49	0.45
1:A:114:ARG:NH2	1:A:174:VAL:HG13	2.30	0.45
1:A:367:VAL:HG12	1:A:369:PHE:CE2	2.51	0.45
1:C:270:VAL:CG2	1:C:413:LEU:CD2	2.92	0.45
1:C:79:SER:HB2	1:C:101:LYS:CE	2.45	0.45
1:D:287:ILE:HG23	1:D:367:VAL:O	2.16	0.45
1:D:267:LYS:HA	1:D:413:LEU:CD2	2.47	0.45
1:A:103:TYR:HE1	1:A:190:ARG:HB2	1.81	0.45
1:A:220:LYS:HD2	1:A:280:ASP:OD2	2.16	0.45
1:B:153:GLU:HG3	1:B:200:MET:HE2	1.98	0.45
1:B:207:PHE:CZ	1:B:284:LEU:HD21	2.51	0.45
1:B:62:LEU:HA	1:B:65:VAL:HG23	1.98	0.45
1:A:266:LEU:CD2	1:A:413:LEU:CD2	2.76	0.45
1:B:89:PHE:CE1	1:C:106:GLN:HG2	2.52	0.45
1:D:174:VAL:O	1:D:177:HIS:ND1	2.50	0.45
1:A:215:ARG:HB2	1:A:287:ILE:CD1	2.40	0.45
1:A:90:HIS:O	1:A:91:ARG:CG	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:O	1:B:170:HIS:N	2.50	0.45
1:C:213:VAL:HG22	1:C:369:PHE:CD2	2.51	0.45
1:C:270:VAL:CG2	1:C:412:PHE:HD2	2.30	0.45
1:D:112:ARG:HG2	1:D:186:LEU:HB3	1.99	0.45
1:D:154:VAL:HG21	1:D:159:ILE:HD11	1.98	0.45
1:B:215:ARG:O	1:B:287:ILE:N	2.46	0.45
1:B:71:LEU:CD1	1:B:107:VAL:HG22	2.47	0.45
1:C:266:LEU:HD21	1:C:412:PHE:CD2	2.52	0.45
1:D:146:ASP:HB3	1:D:148:THR:OG1	2.16	0.45
1:A:62:LEU:CD1	1:D:89:PHE:CZ	3.00	0.45
1:C:81:LYS:HA	1:C:100:PHE:O	2.17	0.45
1:D:63:SER:C	1:D:65:VAL:H	2.19	0.45
1:B:266:LEU:O	1:B:270:VAL:HG23	2.16	0.45
1:B:219:LEU:HD22	1:B:415:PHE:CE2	2.52	0.45
1:C:121:ASP:O	1:C:125:SER:N	2.49	0.45
1:C:175:LYS:HB3	1:C:175:LYS:HE3	1.64	0.45
1:D:179:ASN:N	1:D:179:ASN:OD1	2.50	0.45
1:D:162:MET:HG2	1:D:188:MET:SD	2.56	0.45
1:A:84:VAL:HG22	1:D:82:ILE:HG23	1.98	0.45
1:A:74:ASP:O	1:A:77:LYS:HG2	2.17	0.45
1:B:59:ILE:HG21	1:B:123:LEU:HD13	1.99	0.45
1:B:180:THR:OG1	1:B:182:LEU:HB2	2.16	0.45
1:B:245:PHE:CZ	1:B:415:PHE:CE2	3.05	0.45
1:D:106:GLN:OE1	1:D:109:ARG:NH1	2.50	0.45
1:D:65:VAL:HG12	1:D:109:ARG:HH12	1.80	0.45
1:D:207:PHE:CE2	1:D:216:LYS:HE3	2.51	0.45
1:D:220:LYS:NZ	1:D:280:ASP:CG	2.70	0.45
1:A:266:LEU:HD23	1:A:266:LEU:O	2.16	0.45
1:A:74:ASP:HA	1:A:77:LYS:HG3	1.99	0.45
1:C:215:ARG:NH1	1:C:248:LYS:HZ3	2.15	0.45
1:C:261:ILE:O	1:C:264:GLU:HB2	2.17	0.45
1:D:170:HIS:HA	1:D:173:ILE:HG12	1.98	0.45
1:D:290:ILE:HD12	1:D:366:GLU:HA	1.99	0.45
1:D:283:LEU:HA	1:D:372:LEU:HA	1.99	0.45
1:D:407:GLN:N	1:D:407:GLN:HE21	2.14	0.45
1:A:162:MET:HE1	1:A:185:PHE:CE2	2.52	0.44
1:A:50:VAL:HG21	1:A:193:VAL:HG21	1.98	0.44
1:A:279:MET:HB2	1:A:280:ASP:H	1.66	0.44
1:A:181:LEU:O	1:A:372:LEU:N	2.50	0.44
1:A:281:TYR:CA	1:A:374:ASP:O	2.65	0.44
1:B:54:GLY:HA3	1:B:100:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LYS:O	1:B:82:ILE:HD13	2.17	0.44
1:C:110:ASN:O	1:C:113:ASP:HB3	2.16	0.44
1:C:182:LEU:HD23	1:C:375:ILE:CD1	2.47	0.44
1:C:45:ASP:CG	1:C:46:PRO:HD2	2.38	0.44
1:D:146:ASP:O	1:D:147:ARG:HB2	2.17	0.44
1:D:239:THR:O	1:D:239:THR:HG22	2.16	0.44
1:B:141:PHE:HD1	1:B:141:PHE:HA	1.66	0.44
1:B:375:ILE:CG1	1:B:375:ILE:O	2.65	0.44
1:C:68:PRO:HD3	1:C:106:GLN:NE2	2.33	0.44
1:D:161:ASP:C	1:D:164:SER:HG	2.18	0.44
1:A:273:LEU:HD11	1:A:375:ILE:CB	2.48	0.44
1:A:56:ALA:O	1:A:60:ASN:ND2	2.50	0.44
1:B:133:GLU:HA	1:B:142:LEU:HD23	1.99	0.44
1:C:115:PHE:CD1	1:C:184:GLN:HB3	2.53	0.44
1:C:85:ASN:OD1	1:C:85:ASN:N	2.50	0.44
1:D:219:LEU:N	1:D:283:LEU:O	2.49	0.44
1:D:220:LYS:HE2	1:D:220:LYS:HB3	1.35	0.44
1:A:261:ILE:HD12	1:A:261:ILE:N	2.33	0.44
1:A:86:ASN:CG	1:D:80:SER:HA	2.37	0.44
1:B:273:LEU:HA	1:B:276:LEU:HB2	2.00	0.44
1:C:140:ARG:O	1:C:142:LEU:HG	2.17	0.44
1:C:273:LEU:HD12	1:C:278:ILE:HB	1.99	0.44
1:C:95:PRO:O	1:C:98:PHE:HD1	2.00	0.44
1:D:140:ARG:NE	1:D:153:GLU:OE1	2.50	0.44
1:A:129:ASN:HB3	1:A:145:TYR:CG	2.52	0.44
1:B:158:ASP:OD1	1:B:376:LEU:HD23	2.18	0.44
1:B:45:ASP:CG	1:B:48:VAL:HB	2.37	0.44
1:C:288:HIS:ND1	1:C:367:VAL:HG23	2.33	0.44
1:D:151:ILE:HG23	1:D:202:VAL:HG22	1.99	0.44
1:D:220:LYS:HE3	1:D:281:TYR:O	2.18	0.44
1:D:46:PRO:O	1:D:49:GLY:N	2.50	0.44
1:D:52:LEU:O	1:D:53:TRP:C	2.56	0.44
1:A:212:PRO:HD2	1:A:288:HIS:NE2	2.33	0.44
1:B:122:TYR:O	1:B:126:LEU:HD22	2.18	0.44
1:B:66:PRO:HA	1:B:67:PRO:HD2	1.87	0.44
1:D:71:LEU:HD23	1:D:71:LEU:N	2.32	0.44
1:D:245:PHE:HD1	1:D:250:GLN:HB2	1.83	0.44
1:D:55:VAL:HG11	1:D:126:LEU:CD1	2.44	0.44
1:D:65:VAL:O	1:D:109:ARG:NH2	2.50	0.44
1:A:239:THR:O	1:A:239:THR:HG22	2.18	0.44
1:A:261:ILE:O	1:A:264:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:HD1	1:A:372:LEU:CD1	2.18	0.44
1:C:179:ASN:OD1	1:C:179:ASN:N	2.49	0.44
1:D:170:HIS:HA	1:D:173:ILE:CG1	2.48	0.44
1:A:108:PHE:O	1:A:112:ARG:NH1	2.51	0.43
1:B:142:LEU:HA	1:B:142:LEU:HD23	1.87	0.43
1:B:219:LEU:HD22	1:B:415:PHE:HE2	1.83	0.43
1:B:145:TYR:CZ	1:B:146:ASP:OD1	2.71	0.43
1:D:159:ILE:O	1:D:162:MET:CB	2.66	0.43
1:D:93:ASN:C	1:D:93:ASN:OD1	2.56	0.43
1:B:273:LEU:C	1:B:278:ILE:HB	2.37	0.43
1:C:247:ASN:OD1	1:C:248:LYS:N	2.51	0.43
1:C:287:ILE:CG2	1:C:366:GLU:OE2	2.66	0.43
1:D:109:ARG:O	1:D:112:ARG:HB2	2.19	0.43
1:C:101:LYS:HB2	1:C:190:ARG:HH21	1.83	0.43
1:C:83:LYS:HG3	1:C:99:LYS:HE3	2.01	0.43
1:D:404:HIS:N	1:D:404:HIS:HD1	2.16	0.43
1:D:49:GLY:O	1:D:94:LEU:HD21	2.19	0.43
1:B:170:HIS:O	1:B:174:VAL:HG23	2.17	0.43
1:C:414:ASP:HA	1:C:417:THR:HG22	2.00	0.43
1:C:45:ASP:HA	1:C:46:PRO:HD3	1.60	0.43
1:C:83:LYS:CB	1:C:99:LYS:HE3	2.48	0.43
1:A:373:ILE:O	1:A:375:ILE:N	2.47	0.43
1:D:180:THR:HG22	1:D:268:ARG:HH12	1.83	0.43
1:D:284:LEU:O	1:D:370:MET:HA	2.19	0.43
1:A:220:LYS:HD2	1:A:280:ASP:CG	2.38	0.43
1:A:412:PHE:CE2	1:A:416:ILE:HD12	2.54	0.43
1:A:51:PHE:CZ	1:A:151:ILE:HG21	2.54	0.43
1:A:51:PHE:O	1:A:55:VAL:HG23	2.19	0.43
1:B:243:MET:O	1:B:247:ASN:OD1	2.37	0.43
1:C:129:ASN:HB2	1:C:145:TYR:CD1	2.53	0.43
1:C:158:ASP:OD1	1:C:376:LEU:HD13	2.19	0.43
1:A:285:LEU:HD22	1:A:286:GLY:N	2.33	0.43
1:B:283:LEU:CD2	1:B:370:MET:CE	2.89	0.43
1:C:215:ARG:NH1	1:C:248:LYS:NZ	2.67	0.43
1:C:281:TYR:HA	1:C:374:ASP:HB3	2.01	0.43
1:B:140:ARG:O	1:B:152:LYS:HG3	2.19	0.43
1:B:195:ASN:O	1:B:195:ASN:OD1	2.37	0.43
1:B:207:PHE:CD2	1:B:213:VAL:HG21	2.54	0.43
1:B:54:GLY:HA3	1:B:100:PHE:CD2	2.54	0.43
1:B:54:GLY:O	1:B:57:HIS:N	2.52	0.43
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HH12	1:C:142:LEU:HD21	1.84	0.43
1:C:45:ASP:HB3	1:C:48:VAL:CG1	2.44	0.43
1:D:123:LEU:O	1:D:126:LEU:N	2.50	0.43
1:D:176:CYS:HB2	1:D:268:ARG:NH1	2.34	0.43
1:D:261:ILE:H	1:D:261:ILE:CD1	2.27	0.43
1:D:128:ARG:HE	1:D:128:ARG:HB3	1.69	0.43
1:A:185:PHE:HZ	1:A:375:ILE:HD11	1.84	0.42
1:A:47:LEU:CD1	1:A:198:SER:HB2	2.47	0.42
1:B:70:MET:CE	1:B:72:LEU:HG	2.49	0.42
1:C:126:LEU:HD22	1:C:126:LEU:HA	1.84	0.42
1:C:183:PRO:HB2	1:C:185:PHE:CZ	2.55	0.42
1:C:259:LYS:HZ3	1:C:263:LEU:HD21	1.84	0.42
1:C:270:VAL:CG2	1:C:412:PHE:CD2	3.02	0.42
1:D:159:ILE:HG13	1:D:199:TYR:CD2	2.54	0.42
1:D:162:MET:O	1:D:166:LEU:N	2.50	0.42
1:A:184:GLN:O	1:A:186:LEU:HG	2.20	0.42
1:A:270:VAL:HG22	1:A:281:TYR:CE1	2.54	0.42
1:A:55:VAL:HG12	1:A:59:ILE:HD12	2.00	0.42
1:B:163:HIS:NE2	1:B:188:MET:CE	2.82	0.42
1:B:179:ASN:O	1:B:265:LYS:HG2	2.20	0.42
1:C:278:ILE:HD13	1:C:375:ILE:HG23	2.00	0.42
1:A:141:PHE:N	1:A:151:ILE:O	2.53	0.42
1:A:112:ARG:NH1	1:A:186:LEU:O	2.50	0.42
1:A:162:MET:HB3	1:A:188:MET:HE1	2.02	0.42
1:A:214:HIS:N	1:A:287:ILE:O	2.43	0.42
1:A:56:ALA:C	1:A:60:ASN:HD22	2.22	0.42
1:B:273:LEU:HB2	1:B:278:ILE:HB	2.01	0.42
1:B:86:ASN:HD22	1:B:89:PHE:HB3	1.83	0.42
1:C:124:VAL:O	1:C:124:VAL:HG22	2.19	0.42
1:A:117:ILE:HD13	1:A:186:LEU:CD1	2.49	0.42
1:A:405:PRO:O	1:A:409:ALA:HB2	2.19	0.42
1:A:60:ASN:O	1:A:64:GLN:NE2	2.50	0.42
1:A:65:VAL:HG23	1:D:90:HIS:ND1	2.34	0.42
1:B:405:PRO:O	1:B:409:ALA:HB2	2.19	0.42
1:D:213:VAL:HG22	1:D:287:ILE:H	1.85	0.42
1:A:48:VAL:HG12	1:A:49:GLY:N	2.34	0.42
1:B:277:LYS:CD	1:B:277:LYS:O	2.68	0.42
1:C:273:LEU:HD12	1:C:278:ILE:CB	2.49	0.42
1:C:83:LYS:HB2	1:C:99:LYS:HE3	2.02	0.42
1:D:111:LEU:CD2	1:D:173:ILE:HG21	2.50	0.42
1:B:153:GLU:HB2	1:B:200:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:MET:O	1:B:408:TYR:CE2	2.73	0.42
1:C:201:LEU:HD23	1:C:202:VAL:H	1.83	0.42
1:C:283:LEU:HD12	1:C:372:LEU:HD23	2.01	0.42
1:D:154:VAL:CG2	1:D:159:ILE:HD11	2.50	0.42
1:B:103:TYR:CD1	1:B:188:MET:CG	3.02	0.42
1:C:174:VAL:HG13	1:C:175:LYS:N	2.35	0.42
1:C:270:VAL:CA	1:C:273:LEU:HD23	2.50	0.42
1:C:211:LEU:HD22	1:C:288:HIS:CE1	2.55	0.42
1:A:133:GLU:CB	1:A:142:LEU:HD23	2.49	0.42
1:A:52:LEU:HD23	1:A:126:LEU:O	2.20	0.42
1:D:79:SER:CB	1:D:101:LYS:HE2	2.49	0.42
1:B:207:PHE:CD1	1:B:369:PHE:HB2	2.54	0.42
1:C:143:ILE:HG22	1:C:147:ARG:HA	2.01	0.42
1:D:115:PHE:CZ	1:D:184:GLN:HA	2.55	0.42
1:D:147:ARG:HE	1:D:147:ARG:HB3	1.56	0.42
1:A:81:LYS:HB2	1:D:85:ASN:ND2	2.32	0.41
1:B:366:GLU:O	1:B:368:TYR:CE1	2.73	0.41
1:B:412:PHE:CE1	1:B:416:ILE:HG21	2.55	0.41
1:D:83:LYS:HG3	1:D:99:LYS:HG3	2.01	0.41
1:A:71:LEU:HD22	1:A:75:ASP:OD2	2.20	0.41
1:B:162:MET:O	1:B:166:LEU:HB2	2.20	0.41
1:D:49:GLY:HA2	1:D:52:LEU:HD12	2.01	0.41
1:A:287:ILE:HG12	1:A:368:TYR:CE2	2.54	0.41
1:A:94:LEU:HA	1:A:95:PRO:HD3	1.80	0.41
1:B:102:GLU:OE1	1:B:105:PRO:HB3	2.21	0.41
1:B:169:TYR:CZ	1:B:173:ILE:HD11	2.55	0.41
1:C:258:GLU:H	1:C:258:GLU:HG2	1.51	0.41
1:C:82:ILE:O	1:C:99:LYS:HA	2.21	0.41
1:D:414:ASP:O	1:D:417:THR:HB	2.20	0.41
1:D:99:LYS:HB2	1:D:192:SER:OG	2.21	0.41
1:B:151:ILE:CG1	1:B:202:VAL:HG13	2.47	0.41
1:C:165:ASN:HB2	1:C:276:LEU:CD2	2.47	0.41
1:C:284:LEU:CB	1:C:373:ILE:HG21	2.42	0.41
1:C:45:ASP:CG	1:C:46:PRO:CD	2.88	0.41
1:D:285:LEU:HA	1:D:369:PHE:O	2.21	0.41
1:B:101:LYS:HD3	1:B:190:ARG:HD3	2.01	0.41
1:B:159:ILE:HG23	1:B:163:HIS:NE2	2.35	0.41
1:B:283:LEU:HB2	1:B:412:PHE:CE1	2.55	0.41
1:C:269:ASP:HB3	1:C:372:LEU:HD11	2.03	0.41
1:C:265:LYS:O	1:C:269:ASP:OD1	2.38	0.41
1:D:125:SER:HA	1:D:145:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:VAL:HG21	1:B:98:PHE:CB	2.48	0.41
1:C:268:ARG:NH1	1:C:268:ARG:HG2	2.36	0.41
1:C:270:VAL:C	1:C:273:LEU:HD23	2.41	0.41
1:D:287:ILE:HG12	1:D:368:TYR:HD2	1.85	0.41
1:B:48:VAL:HG12	1:B:49:GLY:N	2.35	0.41
1:B:73:PRO:O	1:B:76:PHE:N	2.52	0.41
1:C:270:VAL:O	1:C:273:LEU:HD23	2.20	0.41
1:D:255:GLY:O	1:D:259:LYS:CB	2.64	0.41
1:D:285:LEU:CD2	1:D:370:MET:HB3	2.40	0.41
1:D:404:HIS:N	1:D:404:HIS:ND1	2.68	0.41
1:A:215:ARG:HB3	1:A:287:ILE:HD12	2.00	0.41
1:C:283:LEU:HD23	1:C:283:LEU:O	2.20	0.41
1:A:190:ARG:HD2	1:A:197:ASP:HB3	2.01	0.41
1:C:270:VAL:HG22	1:C:412:PHE:CD2	2.56	0.41
1:D:169:TYR:CE2	1:D:185:PHE:HD2	2.39	0.41
1:B:217:TYR:CD1	1:B:285:LEU:HD12	2.55	0.41
1:B:65:VAL:HA	1:B:66:PRO:HD2	1.86	0.41
1:C:126:LEU:CD2	1:C:144:SER:CB	2.93	0.41
1:A:59:ILE:HD11	1:A:122:TYR:CE2	2.55	0.40
1:D:65:VAL:O	1:D:65:VAL:HG12	2.20	0.40
1:A:81:LYS:C	1:A:82:ILE:HD13	2.42	0.40
1:B:51:PHE:CZ	1:B:151:ILE:HG21	2.56	0.40
1:D:412:PHE:O	1:D:415:PHE:N	2.54	0.40
1:D:221:GLY:HA2	1:D:415:PHE:CD1	2.56	0.40
1:A:71:LEU:HD13	1:A:107:VAL:HG22	2.02	0.40
1:B:261:ILE:HG22	1:B:265:LYS:HE2	2.04	0.40
1:B:265:LYS:HA	1:B:268:ARG:HE	1.86	0.40
1:B:404:HIS:HA	1:B:405:PRO:HD3	1.79	0.40
1:C:216:LYS:HG2	1:C:239:THR:N	2.36	0.40
1:D:282:SER:OG	1:D:374:ASP:HB2	2.20	0.40
1:A:259:LYS:HG2	1:A:263:LEU:HD11	2.02	0.40
1:B:163:HIS:NE2	1:B:188:MET:HE3	2.36	0.40
1:C:103:TYR:OH	1:C:199:TYR:HE2	2.05	0.40
1:C:115:PHE:CZ	1:C:184:GLN:HB3	2.56	0.40
1:A:372:LEU:HD22	1:A:372:LEU:HA	1.79	0.40
1:B:141:PHE:O	1:B:142:LEU:HG	2.22	0.40
1:B:261:ILE:O	1:B:264:GLU:N	2.54	0.40
1:D:267:LYS:O	1:D:271:GLU:HG3	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	229/392 (58%)	189 (82%)	39 (17%)	1 (0%)	34	66
1	B	240/392 (61%)	203 (85%)	37 (15%)	0	100	100
1	C	233/392 (59%)	197 (84%)	35 (15%)	1 (0%)	34	66
1	D	240/392 (61%)	194 (81%)	45 (19%)	1 (0%)	34	66
All	All	942/1568 (60%)	783 (83%)	156 (17%)	3 (0%)	41	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	375	ILE
1	C	241	ARG
1	A	95	PRO

### 5.3.2 Protein sidechains [i](#)

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	231/348 (66%)	175 (76%)	56 (24%)	0	2
1	B	237/348 (68%)	182 (77%)	55 (23%)	1	2
1	C	233/348 (67%)	181 (78%)	52 (22%)	1	2
1	D	237/348 (68%)	177 (75%)	60 (25%)	0	1
All	All	938/1392 (67%)	715 (76%)	223 (24%)	0	2

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	47	LEU
1	A	48	VAL
1	A	52	LEU
1	A	62	LEU
1	A	65	VAL
1	A	70	MET
1	A	77	LYS
1	A	80	SER
1	A	81	LYS
1	A	96	SER
1	A	97	HIS
1	A	120	GLN
1	A	128	ARG
1	A	141	PHE
1	A	151	ILE
1	A	156	SER
1	A	162	MET
1	A	164	SER
1	A	174	VAL
1	A	176	CYS
1	A	191	VAL
1	A	192	SER
1	A	193	VAL
1	A	195	ASN
1	A	196	GLU
1	A	197	ASP
1	A	201	LEU
1	A	204	ARG
1	A	210	ARG
1	A	216	LYS
1	A	220	LYS
1	A	240	LEU
1	A	242	ASP
1	A	243	MET
1	A	248	LYS
1	A	253	TYR
1	A	268	ARG
1	A	272	PHE
1	A	279	MET
1	A	283	LEU
1	A	285	LEU
1	A	289	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	366	GLU
1	A	367	VAL
1	A	370	MET
1	A	372	LEU
1	A	373	ILE
1	A	374	ASP
1	A	404	HIS
1	A	407	GLN
1	A	408	TYR
1	A	410	LYS
1	A	413	LEU
1	A	416	ILE
1	A	417	THR
1	B	48	VAL
1	B	65	VAL
1	B	70	MET
1	B	71	LEU
1	B	77	LYS
1	B	79	SER
1	B	91	ARG
1	B	92	GLU
1	B	93	ASN
1	B	94	LEU
1	B	109	ARG
1	B	114	ARG
1	B	124	VAL
1	B	126	LEU
1	B	128	ARG
1	B	132	SER
1	B	140	ARG
1	B	141	PHE
1	B	146	ASP
1	B	157	GLU
1	B	164	SER
1	B	165	ASN
1	B	168	ASN
1	B	179	ASN
1	B	180	THR
1	B	189	TYR
1	B	191	VAL
1	B	192	SER
1	B	196	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	201	LEU
1	B	210	ARG
1	B	215	ARG
1	B	216	LYS
1	B	245	PHE
1	B	246	LEU
1	B	247	ASN
1	B	252	VAL
1	B	256	GLU
1	B	260	LYS
1	B	266	LEU
1	B	267	LYS
1	B	274	VAL
1	B	278	ILE
1	B	285	LEU
1	B	289	ASP
1	B	366	GLU
1	B	368	TYR
1	B	370	MET
1	B	373	ILE
1	B	375	ILE
1	B	407	GLN
1	B	408	TYR
1	B	410	LYS
1	B	413	LEU
1	B	416	ILE
1	C	47	LEU
1	C	48	VAL
1	C	62	LEU
1	C	63	SER
1	C	69	VAL
1	C	70	MET
1	C	77	LYS
1	C	79	SER
1	C	80	SER
1	C	85	ASN
1	C	92	GLU
1	C	99	LYS
1	C	109	ARG
1	C	126	LEU
1	C	128	ARG
1	C	132	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	146	ASP
1	C	147	ARG
1	C	149	LEU
1	C	150	VAL
1	C	152	LYS
1	C	156	SER
1	C	163	HIS
1	C	164	SER
1	C	165	ASN
1	C	167	SER
1	C	180	THR
1	C	192	SER
1	C	196	GLU
1	C	203	MET
1	C	210	ARG
1	C	240	LEU
1	C	242	ASP
1	C	243	MET
1	C	251	LYS
1	C	253	TYR
1	C	258	GLU
1	C	268	ARG
1	C	273	LEU
1	C	274	VAL
1	C	276	LEU
1	C	282	SER
1	C	285	LEU
1	C	289	ASP
1	C	369	PHE
1	C	370	MET
1	C	373	ILE
1	C	377	THR
1	C	406	GLU
1	C	408	TYR
1	C	410	LYS
1	C	413	LEU
1	D	45	ASP
1	D	47	LEU
1	D	61	GLU
1	D	62	LEU
1	D	64	GLN
1	D	65	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	70	MET
1	D	77	LYS
1	D	79	SER
1	D	82	ILE
1	D	83	LYS
1	D	85	ASN
1	D	90	HIS
1	D	94	LEU
1	D	109	ARG
1	D	114	ARG
1	D	119	ASP
1	D	120	GLN
1	D	121	ASP
1	D	126	LEU
1	D	128	ARG
1	D	132	SER
1	D	135	GLU
1	D	144	SER
1	D	147	ARG
1	D	153	GLU
1	D	163	HIS
1	D	165	ASN
1	D	166	LEU
1	D	167	SER
1	D	180	THR
1	D	186	LEU
1	D	192	SER
1	D	200	MET
1	D	203	MET
1	D	210	ARG
1	D	213	VAL
1	D	216	LYS
1	D	217	TYR
1	D	220	LYS
1	D	245	PHE
1	D	246	LEU
1	D	250	GLN
1	D	252	VAL
1	D	258	GLU
1	D	266	LEU
1	D	273	LEU
1	D	279	MET

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Mol	Chain	Res	Type
1	D	282	SER
1	D	283	LEU
1	D	284	LEU
1	D	289	ASP
1	D	370	MET
1	D	372	LEU
1	D	373	ILE
1	D	404	HIS
1	D	407	GLN
1	D	408	TYR
1	D	410	LYS
1	D	416	ILE

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

Mol	Chain	Res	Type
1	A	57	HIS
1	A	60	ASN
1	A	184	GLN
1	A	195	ASN
1	A	209	HIS
1	A	404	HIS
1	B	57	HIS
1	B	60	ASN
1	B	64	GLN
1	B	86	ASN
1	B	195	ASN
1	B	247	ASN
1	C	87	HIS
1	C	129	ASN
1	C	163	HIS
1	C	195	ASN
1	D	85	ASN
1	D	87	HIS
1	D	195	ASN
1	D	209	HIS
1	D	214	HIS
1	D	288	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	243/392 (61%)	-0.10	3 (1%) 79 73	24, 58, 114, 158	0
1	B	250/392 (63%)	0.02	12 (4%) 30 21	24, 58, 138, 152	0
1	C	245/392 (62%)	-0.08	10 (4%) 37 27	25, 59, 128, 158	0
1	D	250/392 (63%)	-0.06	9 (3%) 42 32	24, 60, 144, 158	0
All	All	988/1568 (63%)	-0.05	34 (3%) 45 35	24, 59, 136, 158	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	ASN	5.1
1	B	416	ILE	4.7
1	A	405	PRO	4.1
1	A	253	TYR	4.0
1	B	219	LEU	3.6
1	B	255	GLY	3.6
1	B	253	TYR	3.6
1	D	416	ILE	3.4
1	D	212	PRO	3.4
1	B	143	ILE	3.4
1	B	412	PHE	3.3
1	C	368	TYR	3.2
1	C	405	PRO	3.1
1	B	406	GLU	3.0
1	C	151	ILE	2.9
1	C	216	LYS	2.9
1	C	279	MET	2.7
1	D	142	LEU	2.6
1	B	165	ASN	2.6
1	D	413	LEU	2.5
1	C	241	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	217	TYR	2.4
1	D	251	LYS	2.4
1	D	412	PHE	2.4
1	D	134	SER	2.4
1	C	126	LEU	2.4
1	B	69	VAL	2.3
1	B	258	GLU	2.2
1	D	65	VAL	2.2
1	B	413	LEU	2.2
1	C	369	PHE	2.2
1	D	213	VAL	2.2
1	A	240	LEU	2.1
1	B	254	ILE	2.1

## 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.