



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:59 PM GMT

PDB ID : 2G01  
Title : Pyrazoloquinolones as Novel, Selective JNK1 inhibitors  
Authors : Abad-Zapatero, C.  
Deposited on : 2006-02-10  
Resolution : 3.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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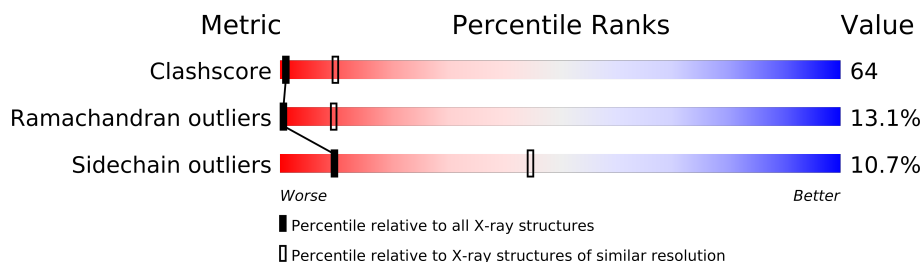
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	
1	B	370	
2	F	11	
2	G	11	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5918 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	1
			2858	1834	482	520	22			
1	B	357	Total	C	N	O	S	0	0	1
			2858	1832	482	522	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	THR	ENGINEEERED	UNP P45983
A	185	GLU	TYR	ENGINEEERED	UNP P45983
A	365	HIS	-	EXPRESSION TAG	UNP P45983
A	366	HIS	-	EXPRESSION TAG	UNP P45983
A	367	HIS	-	EXPRESSION TAG	UNP P45983
A	368	HIS	-	EXPRESSION TAG	UNP P45983
A	369	HIS	-	EXPRESSION TAG	UNP P45983
A	370	HIS	-	EXPRESSION TAG	UNP P45983
B	183	GLU	THR	ENGINEEERED	UNP P45983
B	185	GLU	TYR	ENGINEEERED	UNP P45983
B	365	HIS	-	EXPRESSION TAG	UNP P45983
B	366	HIS	-	EXPRESSION TAG	UNP P45983
B	367	HIS	-	EXPRESSION TAG	UNP P45983
B	368	HIS	-	EXPRESSION TAG	UNP P45983
B	369	HIS	-	EXPRESSION TAG	UNP P45983
B	370	HIS	-	EXPRESSION TAG	UNP P45983

- Molecule 2 is a protein called C-jun-amino-terminal kinase-interacting protein 1.

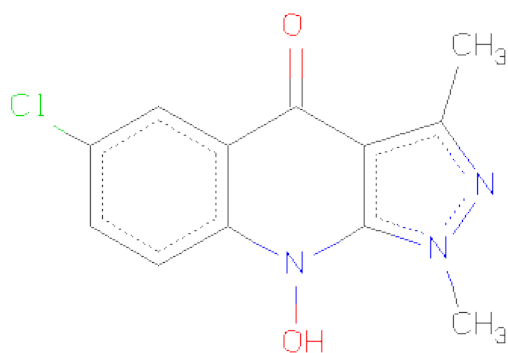
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	1
			73	46	15	12			
2	G	10	Total	C	N	O	0	0	1
			73	46	15	12			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 6-CHLORO-9-HYDROXY-1,3-DIMETHYL-1,9-DIHYDRO-4H-PYRAZOLO[3,4-B]QUINOLIN-4-ONE (three-letter code: 73Q) (formula: C<sub>12</sub>H<sub>10</sub>ClN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			18	12	1	3	2		
4	B	1	Total	C	Cl	N	O	0	0
			18	12	1	3	2		

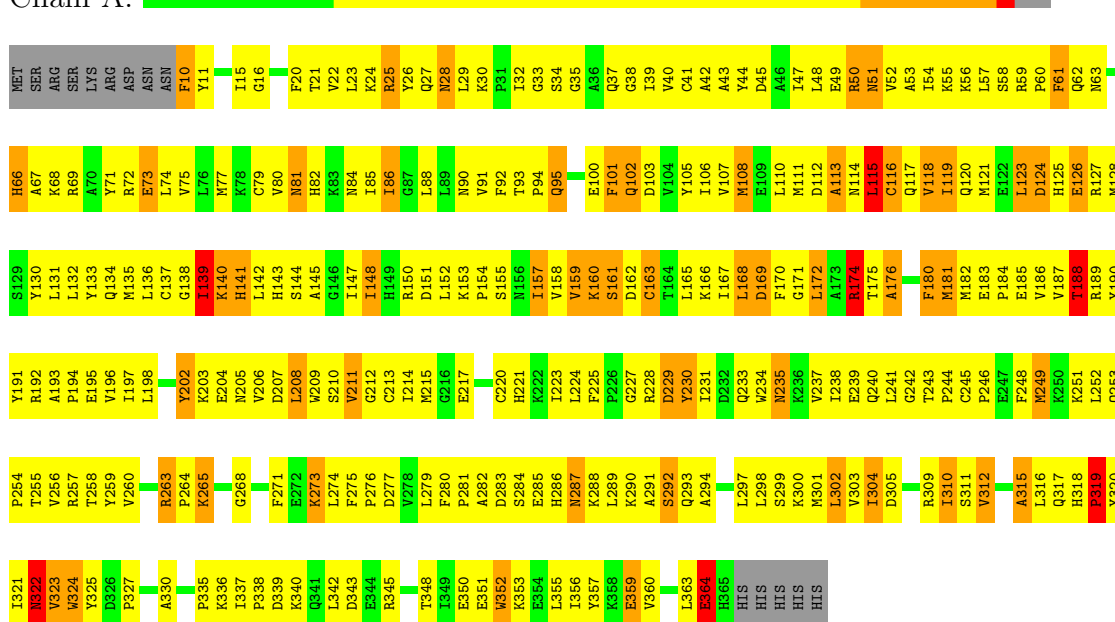
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

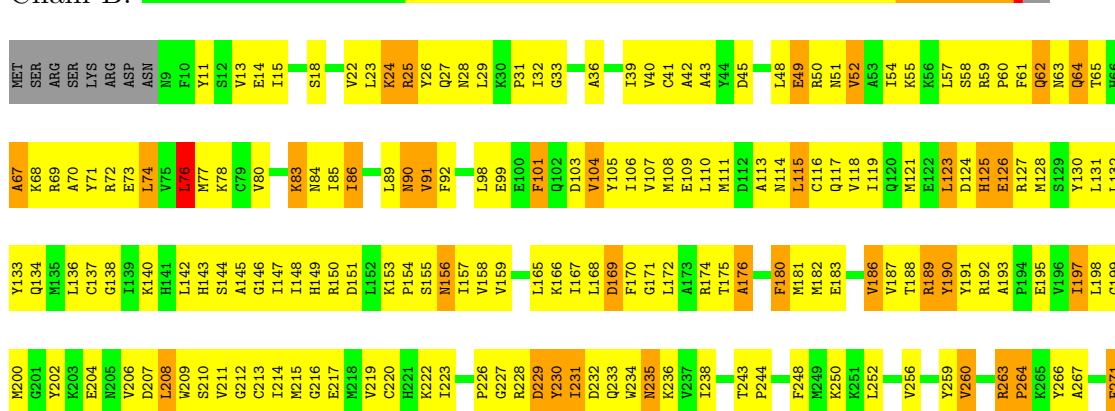
#### • Molecule 1: Mitogen-activated protein kinase 8

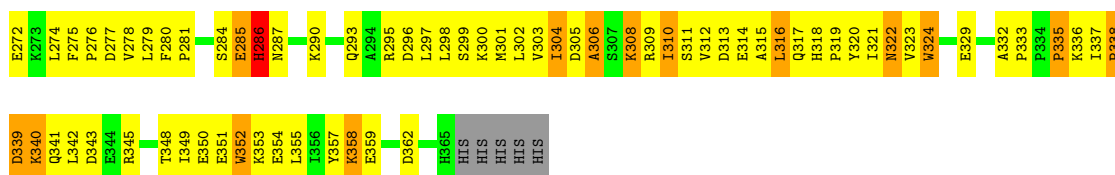
Chain A:



#### • Molecule 1: Mitogen-activated protein kinase 8

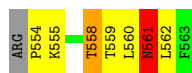
Chain B:





- Molecule 2: C-jun-amino-terminal kinase-interacting protein 1

Chain F:



- Molecule 2: C-jun-amino-terminal kinase-interacting protein 1

Chain G:



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.62Å 150.62Å 119.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 3.50	Depositor
% Data completeness (in resolution range)	77.9 (19.89-3.50)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.283 , 0.354	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5918	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 73Q, SO4

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	0.39	0/2923	0.67	0/3956
1	B	0.41	0/2923	0.69	0/3959
2	F	0.62	0/74	0.87	0/100
2	G	0.58	0/74	0.75	0/100
All	All	0.41	0/5994	0.68	0/8115

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2858	0	2867	423	0
1	B	2858	0	2851	333	0
2	F	73	0	82	7	0
2	G	73	0	82	6	0
3	A	10	0	0	3	0
3	B	10	0	0	1	0
4	A	18	0	10	5	0
4	B	18	0	10	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5918	0	5902	761	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 64.

All (761) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:LEU:HD23	1:A:118:VAL:HG13	1.24	1.12
1:B:304:ILE:HD12	1:B:304:ILE:H	1.08	1.10
1:A:59:ARG:HH21	1:A:66:HIS:HB3	1.14	1.07
1:A:263:ARG:HA	1:A:263:ARG:HH11	1.16	1.06
1:A:115:LEU:HD12	1:A:157:ILE:HG21	1.40	1.04
1:A:263:ARG:NH1	1:A:264:PRO:HD3	1.74	1.02
1:B:348:THR:HB	1:B:351:GLU:H	1.27	0.98
1:A:235:ASN:HD21	1:A:263:ARG:NH2	1.61	0.97
1:A:128:MET:HG2	1:A:132:LEU:HD21	1.48	0.96
1:A:235:ASN:HD21	1:A:263:ARG:HH21	0.96	0.95
1:B:172:LEU:HD21	1:B:186:VAL:HG22	1.46	0.95
1:B:181:MET:HG3	1:B:202:TYR:HE2	1.30	0.95
1:B:57:LEU:HB2	1:B:104:VAL:HG23	1.48	0.94
1:A:142:LEU:H	1:A:142:LEU:HD22	1.32	0.93
1:B:304:ILE:CD1	1:B:304:ILE:H	1.79	0.93
1:B:271:PHE:O	1:B:295:ARG:HD3	1.69	0.92
1:B:318:HIS:ND1	1:B:319:PRO:HD2	1.84	0.92
1:B:51:ASN:HB3	1:B:110:LEU:HD23	1.52	0.91
1:B:215:MET:HE1	1:B:298:LEU:HB2	1.50	0.91
1:B:186:VAL:HG13	1:B:187:VAL:H	1.34	0.91
1:A:189:ARG:HA	1:A:192:ARG:HB2	1.49	0.91
1:A:115:LEU:HD23	1:A:118:VAL:CG1	2.01	0.90
1:A:72:ARG:HD3	1:A:174:ARG:HB3	1.51	0.90
1:A:323:VAL:HG23	1:A:324:TRP:H	1.37	0.89
1:A:263:ARG:HA	1:A:263:ARG:NH1	1.88	0.89
1:B:285:GLU:HG2	1:B:286:HIS:H	1.37	0.88
1:B:153:LYS:HD3	1:B:188:THR:HG21	1.53	0.88
1:B:132:LEU:HD11	1:B:215:MET:HG3	1.56	0.87
1:B:192:ARG:HH22	1:B:230:TYR:HB2	1.38	0.84
1:B:226:PRO:O	1:B:236:LYS:HG3	1.77	0.84
1:A:293:GLN:HG3	1:A:320:TYR:HB2	1.60	0.83
1:A:304:ILE:HD12	1:A:304:ILE:H	1.44	0.83
1:A:189:ARG:HB3	1:A:192:ARG:CZ	2.10	0.82
1:B:304:ILE:HD12	1:B:304:ILE:N	1.92	0.82
1:A:75:VAL:HG21	1:A:340:LYS:HD2	1.60	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:310:ILE:HG12	1:A:311:SER:H	1.42	0.82
1:B:54:ILE:HG12	1:B:107:VAL:HG22	1.62	0.81
1:A:290:LYS:HE3	1:A:292:SER:OG	1.80	0.81
1:B:115:LEU:O	1:B:115:LEU:HD23	1.81	0.81
1:A:59:ARG:HB3	1:A:66:HIS:ND1	1.96	0.80
1:B:181:MET:HG3	1:B:202:TYR:CE2	2.15	0.80
1:B:136:LEU:HB3	1:B:316:LEU:HD11	1.61	0.80
1:A:128:MET:HG2	1:A:132:LEU:CD2	2.11	0.80
1:B:285:GLU:HG2	1:B:286:HIS:N	1.96	0.79
1:A:115:LEU:HB2	1:A:157:ILE:HG22	1.64	0.79
1:A:198:LEU:HD13	1:A:252:LEU:HD21	1.65	0.79
1:A:32:ILE:HG13	1:A:33:GLY:N	1.96	0.79
1:A:111:MET:HB3	1:A:159:VAL:O	1.83	0.79
1:A:235:ASN:ND2	1:A:263:ARG:HH21	1.78	0.79
2:G:555:LYS:HD3	2:G:556:ARG:H	1.48	0.79
1:B:189:ARG:HA	1:B:192:ARG:HD3	1.65	0.78
1:B:227:GLY:HA3	1:B:233:GLN:NE2	1.98	0.78
1:A:174:ARG:HH11	1:A:176:ALA:HB2	1.49	0.77
1:A:115:LEU:C	1:A:117:GLN:H	1.87	0.77
1:B:271:PHE:CE1	1:B:299:SER:HA	2.19	0.77
1:B:189:ARG:NH1	1:B:229:ASP:HA	2.00	0.77
1:A:253:GLN:HB3	1:A:254:PRO:HD2	1.65	0.77
1:B:98:LEU:HD11	1:B:353:LYS:HG2	1.66	0.76
1:B:32:ILE:HG21	1:B:42:ALA:CB	2.16	0.76
1:B:150:ARG:HH21	1:B:181:MET:CG	1.98	0.76
1:A:113:ALA:HA	4:A:901:73Q:H33	1.67	0.76
1:B:136:LEU:HB3	1:B:316:LEU:CD1	2.16	0.75
1:B:172:LEU:HD21	1:B:186:VAL:CG2	2.15	0.75
1:B:132:LEU:O	1:B:136:LEU:HG	1.86	0.75
1:A:59:ARG:NH2	1:A:66:HIS:HB3	1.97	0.75
1:A:10:PHE:HB3	1:A:23:LEU:HA	1.67	0.75
1:B:297:LEU:HB2	1:B:318:HIS:CD2	2.21	0.74
1:B:90:ASN:ND2	1:B:91:VAL:H	1.86	0.73
1:B:32:ILE:HG21	1:B:42:ALA:HB3	1.71	0.73
1:A:125:HIS:HB3	1:A:289:LEU:HD23	1.70	0.73
1:A:38:GLY:HA2	1:A:58:SER:H	1.54	0.73
1:A:286:HIS:O	1:A:287:ASN:HB2	1.88	0.72
1:B:153:LYS:HD3	1:B:188:THR:CG2	2.19	0.72
1:A:318:HIS:HD2	1:A:319:PRO:HD2	1.54	0.72
1:B:148:ILE:HD11	1:B:204:GLU:HG2	1.71	0.72
1:B:217:GLU:OE1	1:B:223:ILE:HA	1.89	0.72
1:B:252:LEU:HD13	1:B:260:VAL:HG21	1.72	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:GLU:O	1:A:50:ARG:HB2	1.90	0.71
1:A:325:TYR:O	1:A:327:PRO:HD3	1.90	0.71
1:B:186:VAL:HG13	1:B:187:VAL:N	2.06	0.71
1:B:192:ARG:HH22	1:B:230:TYR:CB	2.04	0.71
1:A:208:LEU:HD13	1:A:311:SER:HA	1.73	0.70
1:A:142:LEU:CD2	1:A:142:LEU:H	2.05	0.70
1:B:180:PHE:CE2	1:B:199:GLY:HA2	2.26	0.70
1:A:118:VAL:HA	1:A:121:MET:HG3	1.73	0.70
1:A:223:ILE:N	1:A:223:ILE:HD12	2.07	0.70
1:B:116:CYS:O	1:B:119:ILE:HG12	1.91	0.70
1:A:297:LEU:HB2	1:A:318:HIS:HE1	1.56	0.70
1:B:136:LEU:HD13	1:B:315:ALA:HB1	1.74	0.70
1:B:279:LEU:H	1:B:279:LEU:HD12	1.56	0.70
1:B:285:GLU:CG	1:B:286:HIS:H	2.05	0.69
1:A:80:VAL:CG2	1:A:85:ILE:HG21	2.22	0.69
1:B:271:PHE:HZ	1:B:302:LEU:HB2	1.58	0.69
1:A:165:LEU:HD23	1:A:166:LYS:N	2.09	0.68
1:A:275:PHE:CE2	1:A:298:LEU:HD13	2.29	0.68
1:A:139:ILE:HD13	1:A:167:ILE:HD11	1.74	0.68
1:A:168:LEU:N	1:A:168:LEU:HD23	2.09	0.68
1:B:55:LYS:O	1:B:105:TYR:HA	1.93	0.68
1:B:310:ILE:HG13	1:B:314:GLU:HB2	1.74	0.68
1:A:180:PHE:HD1	1:A:181:MET:H	1.40	0.68
1:A:90:ASN:ND2	1:A:91:VAL:H	1.92	0.68
1:B:259:TYR:CE1	1:B:263:ARG:HD3	2.29	0.68
1:A:91:VAL:HG12	1:A:106:ILE:CD1	2.25	0.67
1:A:198:LEU:HD11	1:A:234:TRP:CH2	2.29	0.67
1:A:230:TYR:CE2	1:A:231:ILE:HG13	2.30	0.67
1:B:234:TRP:CE2	1:B:238:ILE:HG21	2.30	0.67
1:B:132:LEU:HD11	1:B:215:MET:CG	2.25	0.67
1:B:271:PHE:CD1	1:B:299:SER:HA	2.28	0.67
1:B:323:VAL:HG23	1:B:324:TRP:N	2.09	0.67
1:A:198:LEU:HD11	1:A:234:TRP:CZ3	2.30	0.67
1:A:244:PRO:HB2	1:A:248:PHE:CD2	2.29	0.67
1:A:273:LYS:HE2	1:A:273:LYS:HA	1.76	0.67
1:A:336:LYS:HG3	1:A:337:ILE:H	1.60	0.67
1:B:150:ARG:HH21	1:B:181:MET:HG2	1.59	0.66
2:G:555:LYS:HD3	2:G:556:ARG:N	2.09	0.66
1:B:290:LYS:HB2	1:B:293:GLN:HB2	1.78	0.66
1:B:11:TYR:OH	1:B:29:LEU:HD21	1.96	0.66
1:A:193:ALA:O	1:A:196:VAL:HB	1.95	0.66
1:B:145:ALA:HB3	1:B:147:ILE:HG13	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:HIS:NE2	1:A:335:PRO:HD3	2.10	0.66
1:A:80:VAL:HG21	1:A:85:ILE:HG21	1.77	0.66
1:B:57:LEU:HD22	1:B:57:LEU:H	1.60	0.66
1:B:305:ASP:HB3	1:B:308:LYS:HE2	1.78	0.66
1:A:244:PRO:HB2	1:A:248:PHE:HD2	1.60	0.66
1:B:180:PHE:CD2	1:B:199:GLY:HA2	2.31	0.66
1:A:187:VAL:O	1:A:187:VAL:HG22	1.96	0.66
1:B:208:LEU:HD12	1:B:310:ILE:HG23	1.78	0.66
1:A:174:ARG:NH1	1:A:176:ALA:HB2	2.10	0.66
1:A:63:ASN:HB2	1:A:66:HIS:CD2	2.30	0.65
1:A:115:LEU:CD1	1:A:157:ILE:HG21	2.23	0.65
1:B:150:ARG:NH2	1:B:181:MET:HG2	2.12	0.65
1:A:56:LYS:HA	1:A:105:TYR:HA	1.78	0.65
1:B:15:ILE:HG22	1:B:15:ILE:O	1.97	0.65
1:B:150:ARG:NH2	1:B:181:MET:SD	2.67	0.65
1:B:192:ARG:HB3	1:B:197:ILE:HG22	1.79	0.65
1:B:137:CYS:HA	1:B:316:LEU:HD21	1.79	0.64
1:B:32:ILE:HD12	1:B:32:ILE:C	2.17	0.64
1:B:123:LEU:HD12	1:B:128:MET:HB2	1.78	0.64
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.62	0.64
1:A:172:LEU:H	1:A:172:LEU:HD23	1.62	0.64
1:A:115:LEU:HB2	1:A:157:ILE:CG2	2.28	0.64
1:A:157:ILE:HD11	1:A:167:ILE:HG12	1.79	0.64
1:B:145:ALA:HB2	1:B:335:PRO:HD2	1.78	0.64
1:B:63:ASN:O	1:B:65:THR:N	2.29	0.64
1:A:352:TRP:HA	1:A:352:TRP:CE3	2.33	0.64
1:A:91:VAL:HG12	1:A:106:ILE:HD12	1.80	0.64
1:B:318:HIS:CG	1:B:319:PRO:HD2	2.33	0.64
1:A:230:TYR:CD2	1:A:231:ILE:HG13	2.33	0.64
1:A:124:ASP:HA	1:A:281:PRO:HB3	1.79	0.63
1:B:86:ILE:HG13	1:B:168:LEU:HD11	1.79	0.63
1:A:309:ARG:O	1:A:310:ILE:O	2.17	0.63
1:A:316:LEU:HA	1:A:321:ILE:HG21	1.80	0.63
1:A:256:VAL:O	1:A:260:VAL:HG23	1.98	0.63
1:B:183:GLU:O	1:B:186:VAL:HG12	1.98	0.62
1:A:183:GLU:C	1:A:185:GLU:H	2.03	0.62
1:B:32:ILE:HD12	1:B:33:GLY:N	2.14	0.62
1:B:157:ILE:N	1:B:157:ILE:HD12	2.14	0.62
1:B:57:LEU:HD23	1:B:104:VAL:HG23	1.81	0.62
1:B:113:ALA:HA	4:B:1001:73Q:H33	1.79	0.62
1:B:352:TRP:HA	1:B:352:TRP:CE3	2.34	0.62
1:A:208:LEU:HD22	1:A:310:ILE:HG23	1.79	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:MET:HG3	1:A:183:GLU:H	1.65	0.62
1:A:115:LEU:N	1:A:157:ILE:O	2.24	0.62
1:B:146:GLY:HA2	1:B:204:GLU:OE2	2.00	0.62
1:A:74:LEU:O	1:A:77:MET:HB2	1.99	0.62
1:A:63:ASN:N	1:A:66:HIS:HE2	1.97	0.62
1:B:148:ILE:HD12	1:B:148:ILE:N	2.15	0.62
1:A:71:TYR:OH	1:A:340:LYS:HD3	1.99	0.62
1:A:143:HIS:ND1	1:A:312:VAL:HG21	2.15	0.62
1:B:60:PRO:O	1:B:67:ALA:HB2	2.00	0.62
1:A:318:HIS:CD2	1:A:319:PRO:HD2	2.33	0.62
1:A:84:ASN:O	1:A:166:LYS:HA	2.00	0.62
1:B:348:THR:HB	1:B:351:GLU:N	2.10	0.62
1:A:304:ILE:H	1:A:304:ILE:CD1	2.02	0.62
1:B:50:ARG:NH2	1:B:89:LEU:HD21	2.15	0.61
1:A:318:HIS:HD2	1:A:319:PRO:CD	2.14	0.61
1:B:227:GLY:HA3	1:B:233:GLN:HE22	1.64	0.61
1:B:149:HIS:O	1:B:150:ARG:HB2	2.01	0.61
1:B:57:LEU:HD11	1:B:106:ILE:HD11	1.83	0.61
1:B:123:LEU:O	1:B:281:PRO:HB3	1.99	0.61
1:A:38:GLY:HA2	1:A:58:SER:N	2.15	0.61
1:A:223:ILE:HG22	1:A:224:LEU:N	2.16	0.61
1:B:165:LEU:C	1:B:165:LEU:HD23	2.21	0.61
1:B:69:ARG:HB3	1:B:171:GLY:O	2.00	0.61
1:A:132:LEU:HD11	1:A:215:MET:HG2	1.82	0.61
1:A:80:VAL:O	1:A:81:ASN:HB2	2.01	0.61
1:B:150:ARG:HD3	1:B:172:LEU:O	2.00	0.61
1:B:114:ASN:O	1:B:116:CYS:N	2.34	0.61
1:B:312:VAL:O	1:B:316:LEU:HD13	2.01	0.61
1:A:220:CYS:O	1:A:221:HIS:HB2	2.01	0.60
1:A:128:MET:O	1:A:132:LEU:HD23	2.01	0.60
1:A:141:HIS:CE1	1:A:335:PRO:HD3	2.37	0.60
1:B:338:PRO:HG2	1:B:340:LYS:HG2	1.83	0.60
1:B:353:LYS:O	1:B:357:TYR:HB3	2.02	0.60
1:B:64:GLN:O	1:B:67:ALA:HB3	2.01	0.60
1:A:198:LEU:HD13	1:A:252:LEU:CD2	2.31	0.60
1:A:115:LEU:O	1:A:117:GLN:N	2.35	0.59
1:A:297:LEU:HB2	1:A:318:HIS:CE1	2.36	0.59
1:A:180:PHE:HD1	1:A:181:MET:N	2.00	0.59
1:B:169:ASP:O	1:B:170:PHE:HB2	2.01	0.59
1:B:219:VAL:O	1:B:279:LEU:HB3	2.01	0.59
1:A:119:ILE:HG13	1:A:217:GLU:HG2	1.84	0.59
1:A:115:LEU:HD22	1:A:119:ILE:HD12	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:157:ILE:HD13	1:A:167:ILE:HA	1.85	0.59
1:A:158:VAL:HG22	1:A:168:LEU:HD22	1.84	0.59
1:A:112:ASP:O	1:A:113:ALA:HB2	2.03	0.59
1:A:125:HIS:O	1:A:126:GLU:C	2.41	0.59
1:B:341:GLN:C	1:B:343:ASP:H	2.05	0.59
1:A:22:VAL:HA	1:A:92:PHE:CZ	2.38	0.59
1:A:115:LEU:C	1:A:117:GLN:N	2.56	0.59
1:A:141:HIS:HB3	1:A:142:LEU:HD22	1.83	0.59
1:B:115:LEU:HB2	1:B:157:ILE:HB	1.84	0.59
1:A:215:MET:SD	1:A:297:LEU:HD23	2.43	0.58
1:A:142:LEU:N	1:A:142:LEU:HD22	2.11	0.58
1:A:186:VAL:HG13	1:A:187:VAL:N	2.18	0.58
1:B:86:ILE:HG13	1:B:168:LEU:CD1	2.33	0.58
1:A:134:GLN:NE2	1:A:163:CYS:O	2.33	0.58
1:A:202:TYR:O	1:A:202:TYR:CD1	2.56	0.58
1:A:10:PHE:HD2	1:A:23:LEU:CD2	2.17	0.58
1:A:119:ILE:CG1	1:A:217:GLU:HG2	2.34	0.58
1:A:234:TRP:NE1	1:A:238:ILE:HG21	2.18	0.58
1:A:22:VAL:HG12	1:A:92:PHE:HZ	1.68	0.58
1:B:23:LEU:O	1:B:25:ARG:N	2.36	0.58
1:A:139:ILE:HD13	1:A:167:ILE:CD1	2.33	0.58
1:B:147:ILE:C	1:B:148:ILE:HD12	2.24	0.58
1:A:350:GLU:O	1:A:353:LYS:HB3	2.03	0.58
1:A:248:PHE:O	1:A:251:LYS:HB2	2.03	0.58
1:A:208:LEU:HD22	1:A:310:ILE:CG2	2.34	0.58
1:A:231:ILE:HD12	1:B:259:TYR:CD2	2.38	0.58
1:A:95:GLN:HG2	1:A:100:GLU:O	2.03	0.58
1:A:352:TRP:O	1:A:356:ILE:HG13	2.03	0.58
1:B:197:ILE:HD11	1:B:234:TRP:HE3	1.69	0.57
1:A:252:LEU:HD12	1:A:252:LEU:N	2.19	0.57
1:A:301:MET:O	1:A:309:ARG:HG3	2.04	0.57
1:B:310:ILE:HG12	1:B:311:SER:N	2.19	0.57
1:A:68:LYS:HG3	1:A:352:TRP:HZ2	1.69	0.57
1:A:223:ILE:N	1:A:223:ILE:CD1	2.67	0.57
1:A:208:LEU:HD23	1:A:301:MET:HE3	1.85	0.57
1:B:275:PHE:CD1	1:B:298:LEU:HD21	2.40	0.57
1:B:153:LYS:CD	1:B:188:THR:HG21	2.29	0.57
1:A:32:ILE:HG12	1:A:40:VAL:O	2.05	0.57
1:A:45:ASP:OD2	1:A:48:LEU:HB3	2.05	0.57
1:B:67:ALA:O	1:B:70:ALA:N	2.38	0.57
1:A:223:ILE:H	1:A:223:ILE:CD1	2.17	0.57
1:B:25:ARG:NH2	1:B:45:ASP:OD2	2.36	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:136:LEU:HD13	1:B:315:ALA:CB	2.34	0.57
1:A:183:GLU:O	1:A:186:VAL:HG12	2.05	0.57
1:B:315:ALA:C	1:B:317:GLN:H	2.09	0.56
1:B:297:LEU:HD13	1:B:318:HIS:CB	2.35	0.56
1:B:323:VAL:CG2	1:B:324:TRP:N	2.67	0.56
1:A:323:VAL:HG23	1:A:324:TRP:N	2.13	0.56
1:A:189:ARG:NE	3:A:501:SO4:S	2.73	0.56
1:A:353:LYS:HA	1:A:356:ILE:HD12	1.87	0.56
1:B:154:PRO:O	1:B:157:ILE:HD12	2.06	0.56
1:A:113:ALA:CA	4:A:901:73Q:H33	2.34	0.56
1:B:296:ASP:OD2	1:B:318:HIS:HE1	1.88	0.56
1:A:160:LYS:O	1:A:162:ASP:OD1	2.24	0.56
1:B:202:TYR:O	1:B:202:TYR:CD1	2.58	0.56
1:B:91:VAL:HG23	1:B:105:TYR:O	2.05	0.56
1:B:114:ASN:C	1:B:116:CYS:H	2.08	0.56
1:A:44:TYR:HB2	1:A:51:ASN:OD1	2.05	0.56
1:A:301:MET:O	1:A:303:VAL:N	2.38	0.56
1:A:176:ALA:HB3	1:A:202:TYR:CE1	2.41	0.56
1:A:304:ILE:O	1:A:305:ASP:C	2.44	0.56
1:B:167:ILE:HG22	1:B:168:LEU:N	2.21	0.56
1:A:315:ALA:O	1:A:318:HIS:HB3	2.06	0.56
1:B:165:LEU:HD23	1:B:166:LYS:N	2.21	0.56
1:A:125:HIS:O	1:A:127:ARG:N	2.39	0.55
1:B:229:ASP:OD1	1:B:232:ASP:N	2.39	0.55
1:B:214:ILE:HG22	1:B:215:MET:N	2.21	0.55
1:A:40:VAL:HA	1:A:54:ILE:O	2.06	0.55
1:A:271:PHE:HA	1:A:274:LEU:HB2	1.89	0.55
1:B:209:TRP:C	1:B:209:TRP:CD1	2.79	0.55
1:A:310:ILE:HG12	1:A:311:SER:N	2.17	0.55
1:A:237:VAL:CG1	1:A:238:ILE:N	2.70	0.55
1:A:108:MET:SD	4:A:901:73Q:H7	2.47	0.55
1:A:25:ARG:O	1:A:45:ASP:HA	2.07	0.55
1:A:242:GLY:N	1:A:268:GLY:HA2	2.22	0.55
1:B:354:GLU:O	1:B:358:LYS:N	2.39	0.55
1:A:264:PRO:O	1:A:265:LYS:O	2.24	0.55
1:B:303:VAL:O	1:B:309:ARG:NH2	2.35	0.55
1:A:50:ARG:O	1:A:52:VAL:HG13	2.06	0.55
1:B:25:ARG:HG2	1:B:26:TYR:CD2	2.40	0.55
1:A:44:TYR:HA	1:A:51:ASN:HA	1.88	0.55
1:B:197:ILE:HD11	1:B:234:TRP:CE3	2.42	0.55
1:B:352:TRP:HE3	1:B:352:TRP:HA	1.71	0.55
1:B:216:GLY:CA	1:B:298:LEU:HD11	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:300:LYS:O	1:B:310:ILE:HG22	2.07	0.54
1:B:323:VAL:HG23	1:B:324:TRP:CD2	2.42	0.54
1:A:68:LYS:HB2	1:A:352:TRP:HE1	1.72	0.54
1:A:242:GLY:H	1:A:268:GLY:HA2	1.71	0.54
1:A:125:HIS:O	1:A:128:MET:N	2.41	0.54
1:B:303:VAL:HB	1:B:309:ARG:HB2	1.90	0.54
1:B:357:TYR:O	1:B:359:GLU:N	2.41	0.54
1:B:15:ILE:HD12	1:B:31:PRO:HG3	1.88	0.54
1:A:114:ASN:HA	1:A:158:VAL:HA	1.90	0.54
1:B:275:PHE:HB3	1:B:280:PHE:CE2	2.43	0.54
1:B:52:VAL:HA	1:B:110:LEU:HB2	1.89	0.54
1:A:243:THR:HG23	1:A:244:PRO:HD2	1.89	0.54
1:A:169:ASP:C	1:A:170:PHE:HD1	2.11	0.54
1:B:348:THR:HB	1:B:351:GLU:HB2	1.89	0.54
1:B:39:ILE:HD12	1:B:39:ILE:N	2.22	0.54
1:B:39:ILE:O	1:B:55:LYS:HA	2.07	0.54
1:A:189:ARG:NE	3:A:501:SO4:O2	2.39	0.54
1:A:195:GLU:H	1:A:195:GLU:CD	2.12	0.54
1:A:304:ILE:N	1:A:304:ILE:HD12	2.19	0.54
1:A:263:ARG:HH12	1:A:264:PRO:HD3	1.69	0.53
1:B:158:VAL:HG23	1:B:166:LYS:HB2	1.90	0.53
1:A:212:GLY:C	1:A:214:ILE:N	2.61	0.53
1:B:202:TYR:O	1:B:202:TYR:HD1	1.92	0.53
1:B:339:ASP:O	1:B:341:GLN:HG3	2.09	0.53
1:B:296:ASP:HB3	1:B:318:HIS:NE2	2.24	0.53
1:B:212:GLY:O	1:B:302:LEU:HD21	2.07	0.53
1:B:136:LEU:CD1	1:B:315:ALA:HB1	2.37	0.53
1:A:32:ILE:CG1	1:A:33:GLY:N	2.68	0.53
1:B:256:VAL:O	1:B:259:TYR:HB3	2.09	0.53
1:A:225:PHE:CE1	1:A:237:VAL:HG23	2.44	0.53
1:A:39:ILE:O	1:A:55:LYS:HA	2.08	0.53
1:B:72:ARG:O	1:B:76:LEU:HB2	2.09	0.53
1:B:189:ARG:NH1	1:B:229:ASP:CA	2.71	0.53
1:B:113:ALA:O	1:B:159:VAL:HG22	2.07	0.53
1:A:157:ILE:O	1:A:157:ILE:HG22	2.08	0.53
1:B:192:ARG:NH2	1:B:230:TYR:HB2	2.18	0.53
1:B:32:ILE:HG23	1:B:42:ALA:H	1.74	0.53
1:A:193:ALA:HB3	1:A:206:VAL:HG23	1.91	0.53
1:A:298:LEU:HD22	1:A:302:LEU:HG	1.89	0.53
1:A:310:ILE:HG23	1:A:311:SER:N	2.22	0.53
1:B:278:VAL:C	1:B:280:PHE:N	2.60	0.53
1:B:117:GLN:HE21	2:G:562:LEU:HB3	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:ASP:O	1:A:125:HIS:HB2	2.08	0.53
1:B:348:THR:CB	1:B:351:GLU:HB2	2.39	0.53
1:A:237:VAL:HG13	1:A:238:ILE:N	2.24	0.53
1:B:114:ASN:OD1	1:B:116:CYS:CB	2.57	0.52
1:A:131:LEU:CD2	1:A:165:LEU:HD12	2.39	0.52
1:A:208:LEU:HD11	1:A:312:VAL:N	2.24	0.52
1:A:298:LEU:O	1:A:301:MET:N	2.34	0.52
1:A:208:LEU:CD1	1:A:311:SER:HA	2.38	0.52
1:A:352:TRP:HA	1:A:352:TRP:HE3	1.72	0.52
1:B:156:ASN:OD1	1:B:169:ASP:HB2	2.09	0.52
1:B:296:ASP:C	1:B:298:LEU:H	2.11	0.52
1:B:309:ARG:O	1:B:310:ILE:O	2.27	0.52
1:B:354:GLU:OE2	1:B:358:LYS:HD2	2.08	0.52
1:B:296:ASP:O	1:B:300:LYS:N	2.41	0.52
1:A:181:MET:C	1:A:183:GLU:H	2.11	0.52
1:B:208:LEU:HD12	1:B:310:ILE:CG2	2.38	0.52
1:B:157:ILE:HG21	1:B:165:LEU:HD11	1.91	0.52
1:A:157:ILE:CD1	1:A:167:ILE:HA	2.40	0.52
1:A:115:LEU:HD12	1:A:157:ILE:CG2	2.27	0.52
1:B:140:LYS:HA	1:B:312:VAL:HG21	1.92	0.52
1:A:112:ASP:HB2	1:A:160:LYS:HA	1.92	0.51
1:B:64:GLN:HG3	1:B:349:ILE:HG22	1.91	0.51
1:B:148:ILE:HG22	1:B:150:ARG:HG3	1.92	0.51
1:A:101:PHE:HD1	1:A:102:GLN:N	2.09	0.51
1:B:50:ARG:HH21	1:B:89:LEU:HD11	1.75	0.51
1:A:29:LEU:O	1:A:30:LYS:HD3	2.09	0.51
1:B:175:THR:O	1:B:176:ALA:O	2.28	0.51
1:A:298:LEU:HD22	1:A:302:LEU:CD1	2.40	0.51
1:B:92:PHE:CE1	1:B:105:TYR:HB2	2.45	0.51
1:A:95:GLN:HG2	1:A:100:GLU:C	2.31	0.51
1:A:93:THR:O	1:A:93:THR:HG23	2.11	0.51
1:B:198:LEU:HD13	1:B:252:LEU:HD22	1.93	0.51
1:B:73:GLU:HG2	1:B:77:MET:HE2	1.92	0.51
1:A:290:LYS:HE3	1:A:292:SER:HG	1.76	0.51
1:A:234:TRP:CE2	1:A:238:ILE:HG21	2.45	0.51
1:A:287:ASN:OD1	1:A:288:LYS:HG3	2.11	0.51
1:B:57:LEU:HD23	1:B:104:VAL:CG2	2.39	0.51
1:B:80:VAL:HG11	1:B:85:ILE:HD13	1.91	0.51
1:A:142:LEU:HB3	1:A:147:ILE:HB	1.92	0.51
1:A:291:ALA:O	1:A:293:GLN:N	2.43	0.51
1:A:195:GLU:CD	1:A:309:ARG:HH22	2.14	0.51
1:A:322:ASN:O	1:A:323:VAL:C	2.49	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:143:HIS:HB2	1:B:312:VAL:HG11	1.92	0.51
1:A:181:MET:C	1:A:183:GLU:N	2.65	0.51
1:A:115:LEU:HA	1:A:118:VAL:CG1	2.41	0.51
1:A:138:GLY:O	1:A:139:ILE:C	2.50	0.51
1:B:316:LEU:N	1:B:316:LEU:HD12	2.26	0.51
1:A:208:LEU:O	1:A:209:TRP:C	2.48	0.50
1:A:318:HIS:CD2	1:A:319:PRO:CD	2.94	0.50
1:B:337:ILE:HG23	1:B:338:PRO:HD2	1.93	0.50
1:A:79:CYS:O	1:A:335:PRO:HB2	2.12	0.50
1:B:357:TYR:C	1:B:359:GLU:H	2.14	0.50
1:A:56:LYS:O	1:A:57:LEU:HB2	2.11	0.50
1:A:209:TRP:O	1:A:210:SER:C	2.49	0.50
1:A:184:PRO:C	1:A:186:VAL:H	2.13	0.50
1:B:154:PRO:O	1:B:156:ASN:N	2.45	0.50
1:A:108:MET:SD	4:A:901:73Q:CL	3.07	0.50
1:A:337:ILE:C	1:A:337:ILE:HD12	2.32	0.50
1:A:189:ARG:HB3	1:A:192:ARG:NH2	2.24	0.50
1:A:255:THR:HG23	3:B:701:SO4:O4	2.12	0.50
1:A:254:PRO:HG2	1:A:255:THR:H	1.76	0.50
1:A:25:ARG:HD2	1:A:47:ILE:HG21	1.92	0.50
1:A:293:GLN:HG3	1:A:320:TYR:CB	2.37	0.50
1:A:311:SER:O	1:A:315:ALA:HB2	2.12	0.50
1:A:21:THR:HB	1:A:94:PRO:HB3	1.92	0.50
1:A:126:GLU:HA	1:A:324:TRP:HH2	1.77	0.50
1:A:153:LYS:HB2	1:A:154:PRO:HD2	1.94	0.50
1:A:287:ASN:C	1:A:289:LEU:H	2.14	0.50
1:A:35:GLY:HA3	1:A:38:GLY:O	2.11	0.50
1:A:47:ILE:O	1:A:47:ILE:HG13	2.12	0.50
1:A:312:VAL:O	1:A:315:ALA:HB3	2.12	0.50
1:B:275:PHE:CE1	1:B:298:LEU:HD21	2.46	0.50
1:A:252:LEU:HD12	1:A:252:LEU:H	1.75	0.50
1:A:245:CYS:O	1:A:248:PHE:HB3	2.11	0.50
1:A:128:MET:O	1:A:132:LEU:CD2	2.60	0.49
1:A:254:PRO:O	1:A:257:ARG:HB3	2.12	0.49
1:B:271:PHE:CZ	1:B:302:LEU:HB2	2.44	0.49
1:A:180:PHE:O	1:A:181:MET:HB2	2.12	0.49
1:A:72:ARG:NH1	1:A:174:ARG:HG2	2.26	0.49
1:B:70:ALA:O	1:B:74:LEU:HB2	2.12	0.49
1:B:167:ILE:CG2	1:B:168:LEU:N	2.74	0.49
1:B:73:GLU:HB2	1:B:171:GLY:HA2	1.95	0.49
1:B:310:ILE:CG1	1:B:314:GLU:HB2	2.39	0.49
1:A:187:VAL:O	1:A:188:THR:C	2.49	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:PHE:CE1	1:A:353:LYS:HE2	2.47	0.49
1:A:88:LEU:HD21	1:A:91:VAL:CG1	2.42	0.49
1:B:259:TYR:OH	1:B:263:ARG:NE	2.45	0.49
1:B:48:LEU:O	1:B:49:GLU:HB2	2.11	0.49
1:A:128:MET:C	1:A:132:LEU:HD23	2.33	0.49
1:A:163:CYS:HA	2:F:560:LEU:HD22	1.93	0.49
1:B:234:TRP:CE2	1:B:238:ILE:CG2	2.95	0.49
1:B:25:ARG:HG2	1:B:26:TYR:CE2	2.48	0.49
1:A:172:LEU:HD23	1:A:172:LEU:N	2.28	0.49
1:A:211:VAL:O	1:A:214:ILE:HB	2.13	0.49
1:B:216:GLY:O	1:B:220:CYS:HB2	2.13	0.49
1:A:107:VAL:O	1:A:108:MET:HB3	2.12	0.49
1:B:29:LEU:HD22	1:B:29:LEU:N	2.28	0.49
1:A:189:ARG:HB3	1:A:192:ARG:NE	2.28	0.49
1:A:27:GLN:O	1:A:28:ASN:C	2.51	0.49
1:A:194:PRO:HD3	1:A:209:TRP:CE2	2.48	0.49
1:A:260:VAL:O	1:A:263:ARG:HG2	2.12	0.49
1:B:319:PRO:HA	1:B:322:ASN:OD1	2.12	0.49
1:B:167:ILE:C	1:B:168:LEU:HD22	2.33	0.49
1:A:160:LYS:O	1:A:160:LYS:HG2	2.13	0.49
1:A:119:ILE:HG22	1:A:120:GLN:HG2	1.95	0.48
1:B:86:ILE:HG21	1:B:108:MET:SD	2.52	0.48
1:A:363:LEU:HD12	1:A:363:LEU:N	2.28	0.48
1:A:94:PRO:HG3	1:A:105:TYR:CE1	2.47	0.48
1:A:183:GLU:C	1:A:185:GLU:N	2.64	0.48
1:A:193:ALA:CB	1:A:206:VAL:HG23	2.43	0.48
1:B:125:HIS:O	1:B:126:GLU:C	2.49	0.48
1:A:135:MET:O	1:A:139:ILE:CD1	2.61	0.48
1:A:135:MET:O	1:A:139:ILE:HG12	2.14	0.48
1:B:274:LEU:HB2	1:B:275:PHE:CD2	2.49	0.48
1:A:325:TYR:HE1	1:A:330:ALA:HB1	1.78	0.48
1:B:68:LYS:O	1:B:71:TYR:HB3	2.13	0.48
1:B:80:VAL:HG11	1:B:85:ILE:CD1	2.44	0.48
2:F:554:PRO:O	2:F:555:LYS:HG3	2.14	0.48
1:B:342:LEU:CD2	1:B:345:ARG:HD3	2.42	0.48
1:A:174:ARG:CZ	1:A:343:ASP:HB3	2.44	0.48
1:A:154:PRO:HD3	1:A:214:ILE:HD13	1.95	0.48
1:A:263:ARG:N	1:A:263:ARG:HD2	2.26	0.48
1:A:174:ARG:HB2	1:A:343:ASP:OD1	2.14	0.48
1:B:114:ASN:OD1	1:B:116:CYS:HB2	2.13	0.48
1:A:208:LEU:HD23	1:A:301:MET:CE	2.42	0.48
1:B:11:TYR:HD1	1:B:24:LYS:HA	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:VAL:HG12	1:A:108:MET:N	2.28	0.48
1:A:162:ASP:HB2	2:F:558:THR:O	2.14	0.48
1:B:332:ALA:HB1	1:B:333:PRO:HD2	1.94	0.48
2:F:561:ASN:C	2:F:561:ASN:HD22	2.16	0.48
1:A:142:LEU:HB3	1:A:147:ILE:CG2	2.43	0.48
1:A:85:ILE:CD1	1:A:167:ILE:HB	2.44	0.48
1:B:317:GLN:HA	1:B:317:GLN:OE1	2.14	0.48
1:A:318:HIS:C	1:A:318:HIS:CD2	2.87	0.48
1:A:62:GLN:N	1:A:66:HIS:HE2	2.12	0.47
1:B:187:VAL:HG13	1:B:192:ARG:CG	2.44	0.47
1:A:32:ILE:HG12	1:A:40:VAL:HG13	1.96	0.47
1:B:108:MET:SD	4:B:1001:73Q:CL	3.09	0.47
1:A:170:PHE:CD1	1:A:170:PHE:N	2.82	0.47
1:A:205:ASN:C	1:A:207:ASP:N	2.68	0.47
1:A:223:ILE:H	1:A:223:ILE:HD12	1.75	0.47
1:A:153:LYS:HE3	1:A:155:SER:HB2	1.96	0.47
1:A:223:ILE:CG2	1:A:224:LEU:N	2.77	0.47
1:B:342:LEU:HD22	1:B:345:ARG:HD3	1.96	0.47
1:A:115:LEU:HD22	1:A:119:ILE:CD1	2.44	0.47
1:A:139:ILE:H	1:A:139:ILE:HD13	1.79	0.47
1:B:238:ILE:HG13	1:B:266:TYR:CD2	2.49	0.47
1:A:230:TYR:CD2	1:A:231:ILE:N	2.82	0.47
1:A:208:LEU:O	1:A:211:VAL:HB	2.15	0.47
1:B:52:VAL:O	1:B:110:LEU:HD22	2.14	0.47
1:B:206:VAL:O	1:B:209:TRP:N	2.46	0.47
1:B:243:THR:HG22	1:B:244:PRO:N	2.30	0.47
1:A:63:ASN:H	1:A:66:HIS:HE2	1.60	0.47
1:A:189:ARG:NE	3:A:501:SO4:O1	2.42	0.47
1:A:353:LYS:O	1:A:356:ILE:HB	2.14	0.47
1:A:130:TYR:O	1:A:133:TYR:HB3	2.14	0.47
1:A:131:LEU:HD23	1:A:165:LEU:HD12	1.95	0.47
1:A:189:ARG:HH12	1:A:227:GLY:C	2.18	0.47
1:A:32:ILE:CG1	1:A:40:VAL:HG13	2.44	0.47
1:A:276:PRO:HD2	1:A:279:LEU:HD12	1.97	0.47
1:A:139:ILE:O	1:A:141:HIS:N	2.48	0.47
1:B:62:GLN:HG2	1:B:63:ASN:OD1	2.14	0.47
1:B:57:LEU:HD21	1:B:106:ILE:HG13	1.97	0.47
1:A:169:ASP:C	1:A:170:PHE:CD1	2.88	0.46
1:A:143:HIS:ND1	1:A:312:VAL:CG2	2.78	0.46
1:B:136:LEU:C	1:B:138:GLY:H	2.19	0.46
1:B:32:ILE:HG21	1:B:42:ALA:HB2	1.95	0.46
1:A:92:PHE:C	1:A:92:PHE:CD1	2.88	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:240:GLN:O	1:A:241:LEU:HD23	2.15	0.46
1:A:280:PHE:CE1	1:A:294:ALA:HB3	2.49	0.46
1:A:81:ASN:O	1:A:82:HIS:HB2	2.14	0.46
1:B:50:ARG:NH2	1:B:109:GLU:HB3	2.30	0.46
1:B:73:GLU:HG2	1:B:77:MET:CE	2.45	0.46
1:A:80:VAL:HG22	1:A:85:ILE:HG21	1.94	0.46
1:B:148:ILE:CD1	1:B:148:ILE:N	2.77	0.46
1:B:216:GLY:HA2	1:B:298:LEU:HD11	1.96	0.46
1:B:286:HIS:O	1:B:287:ASN:HB3	2.15	0.46
1:A:198:LEU:CD1	1:A:252:LEU:HD21	2.38	0.46
1:B:210:SER:O	1:B:213:CYS:HB2	2.16	0.46
1:A:148:ILE:CD1	1:A:175:THR:HA	2.44	0.46
1:A:114:ASN:ND2	1:A:116:CYS:HB3	2.30	0.46
1:B:220:CYS:C	1:B:222:LYS:H	2.19	0.46
1:B:115:LEU:HA	1:B:118:VAL:CG2	2.46	0.46
1:B:305:ASP:O	1:B:306:ALA:C	2.54	0.46
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.68	0.46
1:A:90:ASN:HB3	1:A:107:VAL:HG21	1.96	0.46
1:A:242:GLY:N	1:A:268:GLY:CA	2.78	0.46
1:A:214:ILE:O	1:A:217:GLU:N	2.48	0.46
1:A:183:GLU:N	1:A:184:PRO:CD	2.79	0.46
1:B:71:TYR:OH	1:B:340:LYS:HD2	2.14	0.46
1:B:125:HIS:HD1	1:B:320:TYR:HE1	1.64	0.46
1:B:118:VAL:O	1:B:121:MET:HG2	2.16	0.46
1:A:205:ASN:O	1:A:208:LEU:N	2.46	0.46
1:B:115:LEU:HA	1:B:118:VAL:HG23	1.97	0.46
1:B:123:LEU:HD12	1:B:128:MET:H	1.80	0.46
1:A:238:ILE:HG13	1:A:239:GLU:N	2.30	0.46
1:B:31:PRO:HA	1:B:41:CYS:SG	2.56	0.46
1:A:294:ALA:O	1:A:297:LEU:HB3	2.15	0.46
1:A:342:LEU:O	1:A:343:ASP:HB2	2.14	0.46
1:A:197:ILE:HG22	1:A:198:LEU:HD23	1.97	0.46
1:B:206:VAL:HG13	1:B:207:ASP:N	2.31	0.46
1:A:283:ASP:O	1:A:285:GLU:N	2.49	0.46
1:B:186:VAL:CG1	1:B:187:VAL:H	2.17	0.45
1:B:189:ARG:O	1:B:191:TYR:N	2.48	0.45
1:A:180:PHE:CD1	1:A:181:MET:N	2.77	0.45
1:A:172:LEU:CD2	1:A:172:LEU:N	2.80	0.45
1:B:180:PHE:O	1:B:181:MET:C	2.55	0.45
1:A:230:TYR:HD2	1:A:231:ILE:H	1.60	0.45
1:A:168:LEU:N	1:A:168:LEU:CD2	2.79	0.45
1:B:271:PHE:CD2	1:B:274:LEU:HD12	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:TYR:O	1:B:27:GLN:C	2.55	0.45
1:B:83:LYS:O	1:B:84:ASN:ND2	2.47	0.45
1:A:91:VAL:CG2	1:A:363:LEU:HB2	2.47	0.45
1:B:142:LEU:C	1:B:144:SER:H	2.20	0.45
1:A:90:ASN:HB3	1:A:107:VAL:CG2	2.47	0.45
1:B:263:ARG:HA	1:B:263:ARG:HD2	1.69	0.45
1:A:298:LEU:O	1:A:300:LYS:N	2.49	0.45
1:A:225:PHE:O	1:A:233:GLN:NE2	2.36	0.45
1:A:43:ALA:HB3	1:A:54:ILE:CD1	2.47	0.45
1:A:54:ILE:HD12	1:A:54:ILE:N	2.31	0.45
1:B:357:TYR:C	1:B:359:GLU:N	2.69	0.45
1:A:25:ARG:HB2	1:A:47:ILE:HG22	1.98	0.45
1:B:195:GLU:HB3	1:B:200:MET:HE3	1.97	0.45
1:A:114:ASN:O	1:A:116:CYS:N	2.50	0.45
1:B:131:LEU:O	1:B:132:LEU:C	2.52	0.45
1:B:133:TYR:HB2	1:B:321:ILE:HG23	1.99	0.45
1:A:160:LYS:O	1:A:162:ASP:N	2.50	0.45
1:A:90:ASN:ND2	1:A:91:VAL:N	2.64	0.45
1:A:281:PRO:O	1:A:282:ALA:C	2.55	0.45
1:A:298:LEU:C	1:A:300:LYS:H	2.19	0.45
1:B:142:LEU:HG	1:B:147:ILE:HB	1.98	0.45
1:A:233:GLN:O	1:A:234:TRP:C	2.55	0.45
1:A:225:PHE:CZ	1:A:237:VAL:HG23	2.51	0.45
1:B:13:VAL:HG21	1:B:29:LEU:CD2	2.46	0.45
1:A:220:CYS:O	1:A:221:HIS:CB	2.65	0.45
1:A:133:TYR:O	1:A:136:LEU:HB2	2.16	0.45
1:A:325:TYR:CE1	1:A:330:ALA:HB1	2.53	0.44
1:B:89:LEU:HD11	1:B:109:GLU:HA	1.98	0.44
1:A:86:ILE:HD12	1:A:86:ILE:HA	1.74	0.44
1:B:230:TYR:CE2	1:B:231:ILE:HD11	2.52	0.44
1:B:214:ILE:O	1:B:215:MET:C	2.56	0.44
1:A:342:LEU:O	1:A:342:LEU:HD13	2.17	0.44
1:A:112:ASP:OD1	1:A:161:SER:HB2	2.17	0.44
1:A:165:LEU:HD23	1:A:165:LEU:C	2.37	0.44
1:A:80:VAL:HG22	1:A:81:ASN:H	1.83	0.44
1:B:228:ARG:O	1:B:229:ASP:CB	2.64	0.44
1:B:114:ASN:HD22	4:B:1001:73Q:H12	1.83	0.44
1:A:228:ARG:HG3	1:A:228:ARG:NH1	2.31	0.44
1:A:143:HIS:C	1:A:145:ALA:H	2.21	0.44
1:A:297:LEU:O	1:A:300:LYS:HB2	2.17	0.44
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.83	0.44
1:B:111:MET:HG3	1:B:158:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:67:ALA:O	1:B:68:LYS:C	2.55	0.44
1:B:71:TYR:CE1	1:B:355:LEU:HB3	2.52	0.44
1:B:271:PHE:CZ	1:B:302:LEU:HD12	2.52	0.44
1:A:112:ASP:HB3	2:F:562:LEU:HD12	1.98	0.44
4:A:901:73Q:H31	4:A:901:73Q:O1	2.18	0.44
1:B:89:LEU:HG	1:B:109:GLU:N	2.33	0.44
1:A:29:LEU:HD23	1:A:29:LEU:C	2.38	0.44
1:A:311:SER:O	1:A:315:ALA:N	2.48	0.44
1:A:229:ASP:O	1:A:230:TYR:C	2.56	0.44
1:A:11:TYR:O	1:A:21:THR:HA	2.17	0.44
1:A:293:GLN:NE2	1:A:319:PRO:CB	2.81	0.44
1:B:284:SER:HB3	1:B:285:GLU:H	1.62	0.44
1:A:197:ILE:HD11	1:A:233:GLN:CG	2.47	0.44
1:B:198:LEU:HD13	1:B:252:LEU:CD2	2.47	0.44
1:B:339:ASP:O	1:B:341:GLN:N	2.51	0.44
1:B:117:GLN:NE2	2:G:562:LEU:HB3	2.32	0.44
1:A:119:ILE:HG22	1:A:120:GLN:N	2.32	0.44
1:B:90:ASN:HB3	1:B:107:VAL:HB	2.00	0.44
1:B:296:ASP:HB3	1:B:318:HIS:CE1	2.53	0.44
1:A:246:PRO:HA	1:A:249:MET:HB2	2.00	0.44
1:A:139:ILE:HG23	1:A:152:LEU:HD11	1.99	0.44
1:A:168:LEU:O	1:A:169:ASP:HB3	2.18	0.44
1:A:127:ARG:NH1	2:F:559:THR:O	2.51	0.44
1:B:32:ILE:HG13	1:B:41:CYS:HA	2.00	0.44
1:A:55:LYS:O	1:A:106:ILE:N	2.49	0.44
1:A:24:LYS:C	1:A:26:TYR:H	2.21	0.44
1:A:118:VAL:HA	1:A:121:MET:CG	2.45	0.43
1:B:90:ASN:ND2	1:B:91:VAL:N	2.62	0.43
1:B:148:ILE:CG1	1:B:204:GLU:HA	2.48	0.43
1:B:310:ILE:HD11	1:B:315:ALA:N	2.33	0.43
1:B:123:LEU:HD12	1:B:128:MET:N	2.32	0.43
1:B:154:PRO:C	1:B:156:ASN:N	2.72	0.43
1:A:325:TYR:CE1	1:A:330:ALA:CB	3.01	0.43
1:B:167:ILE:O	1:B:168:LEU:HD22	2.18	0.43
1:A:243:THR:CG2	1:A:244:PRO:HD2	2.48	0.43
1:B:271:PHE:CE2	1:B:302:LEU:HD12	2.53	0.43
1:A:67:ALA:HB3	1:A:352:TRP:HD1	1.83	0.43
1:B:14:GLU:HG2	1:B:14:GLU:O	2.18	0.43
1:B:341:GLN:C	1:B:343:ASP:N	2.71	0.43
1:B:60:PRO:O	1:B:67:ALA:CB	2.64	0.43
1:A:68:LYS:HE2	1:A:72:ARG:NH2	2.34	0.43
1:B:99:GLU:O	1:B:99:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:MET:HG3	1:A:158:VAL:HG23	2.01	0.43
1:A:211:VAL:HA	1:A:214:ILE:HG13	1.99	0.43
1:B:348:THR:HG22	1:B:350:GLU:H	1.83	0.43
1:B:256:VAL:O	1:B:259:TYR:N	2.45	0.43
1:B:124:ASP:OD1	1:B:127:ARG:HD2	2.19	0.43
1:A:118:VAL:O	1:A:119:ILE:C	2.55	0.43
1:A:134:GLN:O	1:A:135:MET:C	2.55	0.43
1:A:293:GLN:NE2	1:A:319:PRO:HB2	2.33	0.43
1:A:82:HIS:HB3	1:A:85:ILE:HB	2.00	0.43
1:A:235:ASN:ND2	1:A:263:ARG:NH2	2.46	0.43
1:B:278:VAL:C	1:B:280:PHE:H	2.21	0.43
1:A:112:ASP:O	1:A:113:ALA:CB	2.66	0.43
1:A:49:GLU:O	1:A:50:ARG:CB	2.64	0.43
1:A:364:GLU:OE1	1:A:364:GLU:HA	2.18	0.43
1:A:114:ASN:O	1:A:117:GLN:N	2.51	0.43
1:B:57:LEU:HD21	1:B:106:ILE:CG1	2.49	0.43
1:B:276:PRO:O	1:B:278:VAL:N	2.44	0.43
1:A:225:PHE:CD1	1:A:237:VAL:HG23	2.53	0.43
1:B:329:GLU:OE1	2:G:556:ARG:NH2	2.50	0.43
1:B:193:ALA:HA	1:B:209:TRP:CD1	2.53	0.43
1:B:131:LEU:C	1:B:133:TYR:N	2.70	0.43
1:B:83:LYS:C	1:B:84:ASN:HD22	2.21	0.43
1:B:101:PHE:CD1	1:B:357:TYR:HD1	2.37	0.43
1:B:243:THR:HG22	1:B:244:PRO:CD	2.49	0.43
1:B:244:PRO:HB3	1:B:248:PHE:CD2	2.54	0.43
1:A:15:ILE:HD12	1:A:20:PHE:CE1	2.54	0.43
1:B:319:PRO:O	1:B:321:ILE:N	2.52	0.43
1:A:32:ILE:HG21	1:A:42:ALA:HB2	2.01	0.43
1:A:37:GLN:O	1:A:58:SER:N	2.51	0.43
1:B:293:GLN:HA	1:B:293:GLN:OE1	2.19	0.43
1:A:259:TYR:CE1	1:A:263:ARG:NE	2.87	0.43
1:B:130:TYR:O	1:B:134:GLN:HG3	2.19	0.43
1:A:244:PRO:CB	1:A:248:PHE:CD2	3.01	0.43
1:A:170:PHE:HD1	1:A:170:PHE:N	2.15	0.42
1:B:172:LEU:N	1:B:172:LEU:HD12	2.34	0.42
1:B:153:LYS:HE2	1:B:156:ASN:HD22	1.83	0.42
1:B:32:ILE:HG13	1:B:40:VAL:O	2.19	0.42
1:A:190:TYR:H	1:A:190:TYR:HD2	1.68	0.42
1:B:151:ASP:O	1:B:151:ASP:OD1	2.37	0.42
1:B:222:LYS:O	1:B:223:ILE:C	2.56	0.42
1:B:296:ASP:OD2	1:B:318:HIS:CE1	2.69	0.42
1:A:189:ARG:C	1:A:191:TYR:N	2.73	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:TYR:HD1	1:A:202:TYR:H	1.68	0.42
1:B:114:ASN:C	1:B:116:CYS:N	2.71	0.42
1:A:21:THR:HB	1:A:94:PRO:CB	2.49	0.42
1:A:127:ARG:O	1:A:128:MET:C	2.58	0.42
1:A:139:ILE:CD1	1:A:139:ILE:H	2.29	0.42
1:A:158:VAL:HG22	1:A:168:LEU:CD2	2.49	0.42
1:B:105:TYR:CD1	1:B:105:TYR:N	2.87	0.42
1:A:72:ARG:HH11	1:A:174:ARG:HG2	1.83	0.42
1:B:121:MET:HG3	1:B:123:LEU:HD23	2.01	0.42
1:B:123:LEU:HD22	1:B:123:LEU:HA	1.69	0.42
1:B:98:LEU:CD1	1:B:353:LYS:HG2	2.42	0.42
1:A:10:PHE:HD2	1:A:23:LEU:HD23	1.83	0.42
4:B:1001:73Q:H31	4:B:1001:73Q:HO1	1.85	0.42
1:B:323:VAL:CG2	1:B:324:TRP:H	2.32	0.42
1:B:338:PRO:O	1:B:339:ASP:HB3	2.19	0.42
1:A:301:MET:O	1:A:309:ARG:HD3	2.19	0.42
1:A:48:LEU:O	1:A:49:GLU:HB2	2.19	0.42
1:A:151:ASP:O	1:A:151:ASP:OD1	2.38	0.42
1:A:117:GLN:OE1	1:A:117:GLN:HA	2.19	0.42
1:A:298:LEU:C	1:A:300:LYS:N	2.73	0.42
1:B:92:PHE:CD1	1:B:92:PHE:C	2.93	0.42
1:B:215:MET:CE	1:B:298:LEU:HD13	2.50	0.42
1:A:53:ALA:HB2	1:A:110:LEU:HD12	2.01	0.42
1:A:321:ILE:O	1:A:322:ASN:C	2.57	0.42
1:B:149:HIS:O	1:B:150:ARG:CB	2.63	0.42
1:A:73:GLU:O	1:A:77:MET:HG2	2.20	0.42
1:A:85:ILE:HA	1:A:85:ILE:HD13	1.77	0.42
1:B:210:SER:O	1:B:213:CYS:N	2.39	0.42
1:B:32:ILE:CG2	1:B:42:ALA:H	2.32	0.42
1:B:235:ASN:HA	1:B:238:ILE:HG12	2.02	0.42
1:B:300:LYS:O	1:B:310:ILE:CG2	2.67	0.42
1:B:211:VAL:HG11	1:B:301:MET:HE2	2.02	0.42
1:A:28:ASN:OD1	1:A:44:TYR:HB3	2.20	0.42
1:A:139:ILE:HG22	1:A:143:HIS:NE2	2.35	0.42
1:B:136:LEU:C	1:B:138:GLY:N	2.73	0.42
1:B:315:ALA:C	1:B:317:GLN:N	2.73	0.42
1:A:356:ILE:O	1:A:359:GLU:HB2	2.20	0.42
1:A:214:ILE:O	1:A:215:MET:C	2.58	0.41
1:B:296:ASP:C	1:B:298:LEU:N	2.74	0.41
1:A:29:LEU:HD21	1:A:41:CYS:SG	2.60	0.41
1:A:182:MET:HG2	1:B:182:MET:SD	2.60	0.41
1:A:291:ALA:C	1:A:293:GLN:H	2.23	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:54:ILE:HA	1:B:106:ILE:O	2.19	0.41
1:A:101:PHE:CD2	1:A:357:TYR:CD1	3.08	0.41
1:A:61:PHE:CZ	1:A:102:GLN:HA	2.55	0.41
1:A:357:TYR:C	1:A:359:GLU:H	2.23	0.41
1:A:68:LYS:HE2	1:A:72:ARG:HH21	1.84	0.41
1:A:170:PHE:O	1:A:172:LEU:N	2.53	0.41
1:A:256:VAL:HG12	1:A:260:VAL:CG2	2.50	0.41
1:B:169:ASP:HB3	1:B:170:PHE:H	1.69	0.41
1:A:139:ILE:O	1:A:140:LYS:C	2.59	0.41
1:A:297:LEU:CB	1:A:318:HIS:HE1	2.27	0.41
1:B:111:MET:HG3	1:B:158:VAL:CG2	2.51	0.41
1:A:84:ASN:HA	1:A:165:LEU:O	2.20	0.41
1:B:195:GLU:HB3	1:B:200:MET:CE	2.50	0.41
1:A:134:GLN:OE1	1:A:165:LEU:N	2.49	0.41
1:B:297:LEU:O	1:B:301:MET:HB2	2.20	0.41
1:B:13:VAL:HG21	1:B:29:LEU:HD21	2.01	0.41
1:B:310:ILE:HG12	1:B:311:SER:O	2.21	0.41
1:A:102:GLN:O	1:A:103:ASP:CG	2.58	0.41
1:B:26:TYR:O	1:B:43:ALA:HB1	2.20	0.41
1:A:184:PRO:HB2	1:A:192:ARG:NH1	2.36	0.41
1:A:234:TRP:O	1:A:237:VAL:HG12	2.20	0.41
1:A:234:TRP:CD1	1:A:238:ILE:HD13	2.55	0.41
1:B:45:ASP:OD1	1:B:48:LEU:N	2.48	0.41
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.81	0.41
1:A:71:TYR:CE1	1:A:355:LEU:HB3	2.56	0.41
1:A:197:ILE:HG22	1:A:198:LEU:N	2.34	0.41
1:A:53:ALA:HB3	1:A:108:MET:HG3	2.03	0.41
1:A:38:GLY:CA	1:A:58:SER:H	2.28	0.41
1:A:223:ILE:HG22	1:A:224:LEU:H	1.85	0.41
1:B:60:PRO:HG2	1:B:61:PHE:H	1.86	0.41
1:B:190:TYR:HB2	1:B:191:TYR:CE1	2.55	0.41
1:B:136:LEU:HB3	1:B:316:LEU:HD12	1.98	0.41
1:B:297:LEU:HD13	1:B:318:HIS:CG	2.56	0.41
1:A:351:GLU:HG2	1:A:355:LEU:CD1	2.51	0.41
1:B:209:TRP:O	1:B:209:TRP:CD1	2.73	0.41
2:F:561:ASN:ND2	2:F:561:ASN:C	2.74	0.41
1:B:244:PRO:CB	1:B:248:PHE:CD2	3.04	0.41
1:A:212:GLY:O	1:A:214:ILE:N	2.54	0.40
1:A:139:ILE:CD1	1:A:167:ILE:HD11	2.47	0.40
1:A:280:PHE:HA	1:A:281:PRO:HD3	1.97	0.40
1:A:264:PRO:O	1:A:265:LYS:C	2.60	0.40
1:B:149:HIS:HE1	1:B:151:ASP:HB3	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:130:TYR:CZ	2:G:556:ARG:HD3	2.55	0.40
1:A:253:GLN:HB3	1:A:254:PRO:CD	2.43	0.40
1:A:245:CYS:HA	1:A:246:PRO:HD3	1.85	0.40
1:B:208:LEU:HA	1:B:208:LEU:HD22	1.82	0.40
1:A:224:LEU:HA	1:A:224:LEU:HD12	1.84	0.40
1:A:263:ARG:HA	1:A:264:PRO:HD3	1.93	0.40
1:B:84:ASN:OD1	1:B:137:CYS:SG	2.76	0.40
1:B:51:ASN:O	1:B:52:VAL:HG13	2.22	0.40
1:A:186:VAL:HG13	1:A:187:VAL:H	1.85	0.40
1:B:14:GLU:O	1:B:15:ILE:HD13	2.22	0.40
1:A:135:MET:HG2	1:A:139:ILE:HD11	2.02	0.40
1:A:137:CYS:O	1:A:140:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	354/370 (96%)	213 (60%)	92 (26%)	49 (14%)	0	8
1	B	355/370 (96%)	229 (64%)	81 (23%)	45 (13%)	0	10
2	F	8/11 (73%)	6 (75%)	1 (12%)	1 (12%)	1	10
2	G	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
All	All	725/762 (95%)	454 (63%)	176 (24%)	95 (13%)	0	9

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	50	ARG
1	A	60	PRO
1	A	123	LEU
1	A	126	GLU
1	A	161	SER

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Mol	Chain	Res	Type
1	A	181	MET
1	A	265	LYS
1	A	287	ASN
1	A	302	LEU
1	A	310	ILE
1	A	319	PRO
1	A	322	ASN
1	A	323	VAL
1	B	24	LYS
1	B	36	ALA
1	B	115	LEU
1	B	176	ALA
1	B	189	ARG
1	B	190	TYR
1	B	308	LYS
1	B	310	ILE
1	B	339	ASP
1	A	16	GLY
1	A	28	ASN
1	A	81	ASN
1	A	113	ALA
1	A	116	CYS
1	A	140	LYS
1	A	141	HIS
1	A	144	SER
1	A	163	CYS
1	A	188	THR
1	A	203	LYS
1	A	204	GLU
1	A	292	SER
1	A	338	PRO
1	A	348	THR
1	A	364	GLU
1	B	18	SER
1	B	58	SER
1	B	62	GLN
1	B	74	LEU
1	B	83	LYS
1	B	86	ILE
1	B	126	GLU
1	B	155	SER
1	B	229	ASP

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Mol	Chain	Res	Type
1	B	231	ILE
1	B	267	ALA
1	B	286	HIS
1	B	306	ALA
1	B	322	ASN
1	B	340	LYS
1	B	358	LYS
1	A	102	GLN
1	A	115	LEU
1	A	160	LYS
1	A	171	GLY
1	A	299	SER
2	F	561	ASN
1	B	25	ARG
1	B	49	GLU
1	B	101	PHE
1	B	125	HIS
1	B	186	VAL
1	B	235	ASN
1	B	264	PRO
1	B	336	LYS
1	A	25	ARG
1	A	174	ARG
1	A	176	ALA
1	A	229	ASP
1	A	339	ASP
1	B	78	LYS
1	B	169	ASP
1	A	108	MET
1	A	169	ASP
1	A	315	ALA
1	B	64	GLN
1	B	67	ALA
1	B	91	VAL
1	B	277	ASP
1	B	316	LEU
1	A	235	ASN
1	A	284	SER
1	B	76	LEU
1	B	250	LYS
1	A	139	ILE
1	A	211	VAL

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Mol	Chain	Res	Type
1	A	360	VAL
1	B	260	VAL
1	A	159	VAL
1	B	335	PRO
1	B	338	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/334 (94%)	274 (87%)	41 (13%)	6	33
1	B	314/334 (94%)	288 (92%)	26 (8%)	16	59
2	F	9/11 (82%)	7 (78%)	2 (22%)	1	8
2	G	9/11 (82%)	9 (100%)	0	100	100
All	All	647/690 (94%)	578 (89%)	69 (11%)	10	45

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	51	ASN
1	A	61	PHE
1	A	66	HIS
1	A	69	ARG
1	A	73	GLU
1	A	86	ILE
1	A	95	GLN
1	A	101	PHE
1	A	115	LEU
1	A	118	VAL
1	A	119	ILE
1	A	124	ASP
1	A	139	ILE
1	A	148	ILE
1	A	150	ARG
1	A	157	ILE

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	172	LEU
1	A	174	ARG
1	A	180	PHE
1	A	188	THR
1	A	202	TYR
1	A	208	LEU
1	A	213	CYS
1	A	230	TYR
1	A	249	MET
1	A	258	THR
1	A	263	ARG
1	A	273	LYS
1	A	277	ASP
1	A	304	ILE
1	A	312	VAL
1	A	317	GLN
1	A	319	PRO
1	A	322	ASN
1	A	324	TRP
1	A	345	ARG
1	A	352	TRP
1	A	359	GLU
1	A	364	GLU
2	F	558	THR
2	F	561	ASN
1	B	22	VAL
1	B	28	ASN
1	B	52	VAL
1	B	59	ARG
1	B	76	LEU
1	B	90	ASN
1	B	103	ASP
1	B	104	VAL
1	B	123	LEU
1	B	156	ASN
1	B	174	ARG
1	B	180	PHE
1	B	197	ILE
1	B	208	LEU
1	B	230	TYR
1	B	263	ARG

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Mol	Chain	Res	Type
1	B	264	PRO
1	B	271	PHE
1	B	272	GLU
1	B	285	GLU
1	B	286	HIS
1	B	304	ILE
1	B	313	ASP
1	B	324	TRP
1	B	352	TRP
1	B	362	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	37	GLN
1	A	84	ASN
1	A	90	ASN
1	A	120	GLN
1	A	235	ASN
1	A	317	GLN
1	A	322	ASN
2	F	561	ASN
1	B	28	ASN
1	B	37	GLN
1	B	90	ASN
1	B	102	GLN
1	B	117	GLN
1	B	141	HIS
1	B	233	GLN
1	B	318	HIS
1	B	347	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	A	501	-	4,4,4	1.37	0	6,6,6	0.06	0
3	SO4	A	601	-	4,4,4	0.98	0	6,6,6	0.12	0
4	73Q	A	901	-	20,20,20	2.16	6 (30%)	22,31,31	2.25	9 (40%)
4	73Q	B	1001	-	20,20,20	2.05	5 (25%)	22,31,31	2.17	7 (31%)
3	SO4	B	701	-	4,4,4	1.33	0	6,6,6	0.09	0
3	SO4	B	801	-	4,4,4	1.12	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	501	-	-	0/0/0/0	0/0/0/0
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
4	73Q	A	901	-	-	0/0/0/0	0/0/3/3
4	73Q	B	1001	-	-	0/0/0/0	0/0/3/3
3	SO4	B	701	-	-	0/0/0/0	0/0/0/0
3	SO4	B	801	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	73Q	C4-N2	-5.20	1.31	1.36
4	A	901	73Q	C4-N2	-5.17	1.31	1.36
4	B	1001	73Q	C4-N3	3.59	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	73Q	C7-C8	3.29	1.44	1.38
4	A	901	73Q	C11-C10	3.22	1.45	1.40
4	B	1001	73Q	C7-C8	3.01	1.43	1.38
4	A	901	73Q	C4-N3	2.93	1.40	1.38
4	A	901	73Q	O2-C11	2.90	1.28	1.23
4	B	1001	73Q	C8-CL	-2.42	1.68	1.74
4	B	1001	73Q	C11-C10	2.35	1.44	1.40
4	A	901	73Q	O1-N3	-2.25	1.35	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	73Q	C2-N1-N2	5.44	109.03	104.35
4	A	901	73Q	C2-N1-N2	5.30	108.91	104.35
4	A	901	73Q	C6-C5-N3	4.51	126.03	119.34
4	B	1001	73Q	C6-C5-N3	4.44	125.92	119.34
4	A	901	73Q	C6-C5-C10	-3.47	114.94	119.94
4	A	901	73Q	C3-N2-N1	3.37	124.50	120.78
4	B	1001	73Q	C6-C5-C10	-3.28	115.21	119.94
4	A	901	73Q	C7-C6-C5	3.18	124.55	119.34
4	B	1001	73Q	C7-C6-C5	2.98	124.21	119.34
4	B	1001	73Q	C3-N2-N1	2.96	124.06	120.78
4	A	901	73Q	C1-C2-N1	2.64	125.39	119.61
4	A	901	73Q	C7-C8-C9	-2.50	118.14	121.93
4	B	1001	73Q	C1-C2-N1	2.49	125.07	119.61
4	B	1001	73Q	C7-C8-C9	-2.07	118.79	121.93
4	A	901	73Q	C5-N3-C4	2.04	122.69	120.16
4	A	901	73Q	C7-C8-CL	2.04	122.71	119.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.