



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 AM GMT

PDB ID : 2F7K  
Title : Crystal Structure of Human Pyridoxal Kinase  
Authors : Jiang, T.; Cao, P.; Gong, Y.; Tang, L.  
Deposited on : 2005-12-01  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

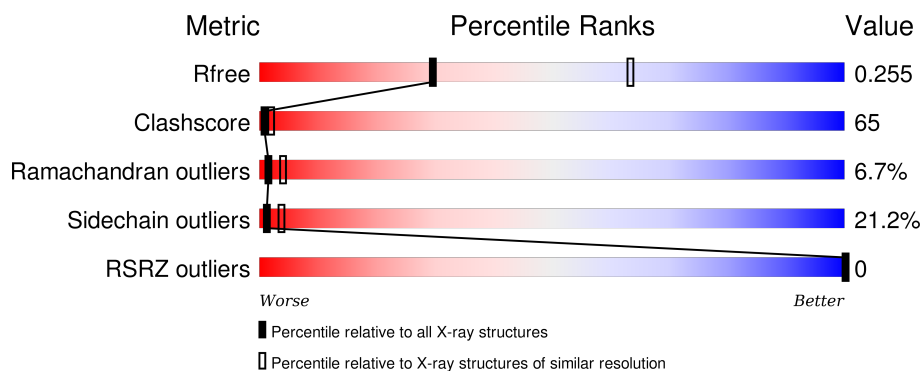
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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	327	 21% 59% 16% ..
1	B	327	 26% 57% 15% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5327 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 Pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2560	1608	458	478	16			
1	B	323	Total	C	N	O	S	0	0	0
			2560	1608	458	478	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	SER	-	CLONING ARTIFACT	UNP O00764
A	-13	TYR	-	CLONING ARTIFACT	UNP O00764
A	-12	TYR	-	CLONING ARTIFACT	UNP O00764
A	-11	HIS	-	EXPRESSION TAG	UNP O00764
A	-10	HIS	-	EXPRESSION TAG	UNP O00764
A	-9	HIS	-	EXPRESSION TAG	UNP O00764
A	-8	HIS	-	EXPRESSION TAG	UNP O00764
A	-7	HIS	-	EXPRESSION TAG	UNP O00764
A	-6	HIS	-	EXPRESSION TAG	UNP O00764
A	-5	HIS	-	EXPRESSION TAG	UNP O00764
A	-4	GLU	-	CLONING ARTIFACT	UNP O00764
A	-3	GLY	-	CLONING ARTIFACT	UNP O00764
A	-2	VAL	-	CLONING ARTIFACT	UNP O00764
A	-1	ARG	-	CLONING ARTIFACT	UNP O00764
A	0	THR	-	CLONING ARTIFACT	UNP O00764
B	-14	SER	-	CLONING ARTIFACT	UNP O00764
B	-13	TYR	-	CLONING ARTIFACT	UNP O00764
B	-12	TYR	-	CLONING ARTIFACT	UNP O00764
B	-11	HIS	-	EXPRESSION TAG	UNP O00764
B	-10	HIS	-	EXPRESSION TAG	UNP O00764
B	-9	HIS	-	EXPRESSION TAG	UNP O00764
B	-8	HIS	-	EXPRESSION TAG	UNP O00764
B	-7	HIS	-	EXPRESSION TAG	UNP O00764
B	-6	HIS	-	EXPRESSION TAG	UNP O00764
B	-5	HIS	-	EXPRESSION TAG	UNP O00764

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLU	-	CLONING ARTIFACT	UNP O00764
B	-3	GLY	-	CLONING ARTIFACT	UNP O00764
B	-2	VAL	-	CLONING ARTIFACT	UNP O00764
B	-1	ARG	-	CLONING ARTIFACT	UNP O00764
B	0	THR	-	CLONING ARTIFACT	UNP O00764

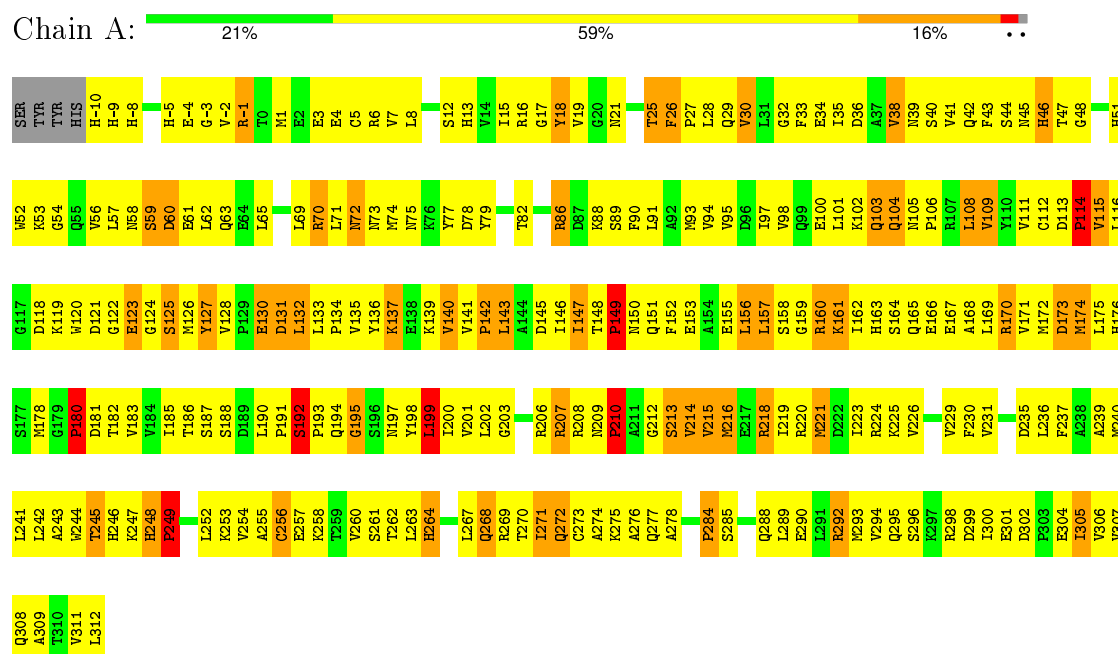
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	96	Total O 96 96	0	0
2	B	111	Total O 111 111	0	0

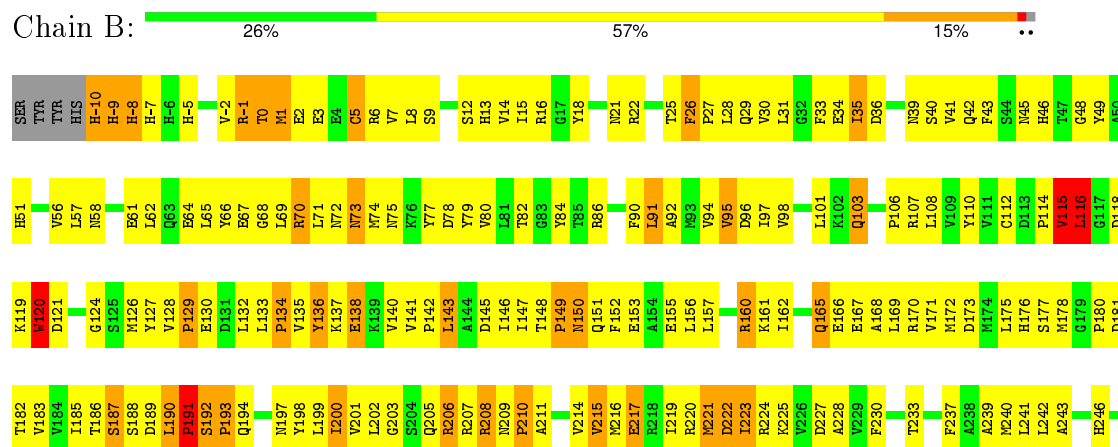
### 3 Residue-property plots

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.

#### • Molecule 1: Pyridoxal kinase



#### • Molecule 1: Pyridoxal kinase



P249	P250	P251	P252	P253		Q256	E257	P258	T259	V260	S261	T262	L263	H264	H265	V266	L267	Q268	P269	T270	L271	Q272	P273	A274		A278	G279	E280	Q281	V282	R283	P284	S285	P286	M287	Q288	L289		R292	M293	V294	Q295	S296	R297	R298	P299	I300	E301	D302	F303	E304	I305	V306	V307	Q308	A309	P310	V311	L312
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.50 Å 52.50 Å 301.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 7.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.0 (8.00-2.80) 81.0 (7.99-2.80)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.94 (at 2.78 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.271 0.213 , 0.255	Depositor DCC
$R_{free}$ test set	707 reflections (4.58%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 71.6	EDS
Estimated twinning fraction	0.190 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 15454 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.46	0/2612	0.87	10/3540 (0.3%)
1	B	0.45	0/2612	0.83	3/3540 (0.1%)
All	All	0.45	0/5224	0.85	13/7080 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	PRO	CA-N-CD	-7.94	100.39	111.50
1	A	149	PRO	CA-N-CD	-7.75	100.66	111.50
1	B	120	TRP	CA-CB-CG	6.54	126.12	113.70
1	A	-3	GLY	N-CA-C	-6.51	96.83	113.10
1	A	192	SER	N-CA-C	-5.85	95.22	111.00
1	B	150	ASN	N-CA-C	-5.79	95.37	111.00
1	A	38	VAL	N-CA-C	-5.60	95.87	111.00
1	A	304	GLU	N-CA-C	-5.49	96.17	111.00
1	A	-4	GLU	N-CA-C	-5.20	96.96	111.00
1	A	150	ASN	N-CA-C	-5.19	96.99	111.00
1	B	116	LEU	N-CA-C	5.18	124.99	111.00
1	A	132	LEU	N-CA-C	5.11	124.81	111.00
1	A	199	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2551	354	0
1	B	2560	0	2551	334	0
2	A	96	0	0	0	0
2	B	111	0	0	3	0
All	All	5327	0	5102	660	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 65.

All (660) 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:A:199:LEU:HB2	1:A:223:ILE:HB	1.38	1.05
1:A:72:ASN:HD21	1:A:74:MET:HG3	1.22	1.04
1:A:221:MET:HG2	1:A:309:ALA:HA	1.39	1.02
1:A:147:ILE:H	1:A:147:ILE:CD1	1.74	1.00
1:A:147:ILE:H	1:A:147:ILE:HD13	1.24	1.00
1:A:230:PHE:HE1	1:A:267:LEU:HB3	1.30	0.97
1:B:162:ILE:HD11	1:B:171:VAL:CG2	1.95	0.96
1:A:35:ILE:H	1:A:35:ILE:HD12	1.28	0.96
1:A:26:PHE:HB3	1:A:27:PRO:HD3	1.49	0.94
1:B:189:ASP:O	1:B:191:PRO:HD3	1.67	0.94
1:A:108:LEU:HG	1:A:109:VAL:H	1.33	0.93
1:A:181:ASP:HB2	1:A:207:ARG:NH2	1.84	0.93
1:A:263:LEU:O	1:A:267:LEU:HG	1.70	0.92
1:A:72:ASN:ND2	1:A:74:MET:HG3	1.85	0.90
1:B:84:TYR:HA	1:B:115:VAL:HB	1.52	0.89
1:B:253:LYS:O	1:B:257:GLU:HG3	1.71	0.89
1:B:311:VAL:HG21	2:B:396:HOH:O	1.73	0.88
1:A:254:VAL:HA	1:A:257:GLU:HB2	1.58	0.86
1:A:197:ASN:C	1:A:225:LYS:HD3	1.97	0.85
1:B:15:ILE:HD11	1:B:42:GLN:HE21	1.42	0.85
1:A:147:ILE:HD12	1:A:180:PRO:HB3	1.60	0.84
1:A:264:HIS:ND1	1:A:306:VAL:HG21	1.92	0.84
1:B:168:ALA:O	1:B:172:MET:HG3	1.77	0.83
1:A:170:ARG:HB2	1:A:170:ARG:CZ	2.07	0.83
1:B:160:ARG:HD2	1:B:161:LYS:H	1.44	0.83
1:B:165:GLN:HG3	1:B:220:ARG:NH1	1.93	0.83
1:A:152:PHE:CE1	1:A:156:LEU:HG	2.14	0.82
1:B:172:MET:HE1	1:B:202:LEU:HD22	1.61	0.82
1:A:4:GLU:HB3	1:A:6:ARG:HG3	1.61	0.82
1:A:8:LEU:HB2	1:A:77:TYR:CE2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HA	1:A:272:GLN:HB2	1.62	0.81
1:A:112:CYS:SG	1:A:114:PRO:HD3	2.22	0.80
1:B:210:PRO:HG2	1:B:215:VAL:CG1	2.11	0.80
1:B:278:ALA:HB2	1:B:288:GLN:NE2	1.97	0.79
1:A:147:ILE:CD1	1:A:147:ILE:N	2.45	0.79
1:A:230:PHE:CE1	1:A:267:LEU:HB3	2.18	0.79
1:A:181:ASP:HB2	1:A:207:ARG:HH21	1.44	0.79
1:A:220:ARG:C	1:A:221:MET:HG3	2.03	0.79
1:B:205:GLN:CB	1:B:252:LEU:HD11	2.13	0.79
1:B:26:PHE:O	1:B:30:VAL:HG12	1.83	0.78
1:B:90:PHE:O	1:B:94:VAL:HG23	1.83	0.78
1:A:254:VAL:HG12	1:A:258:LYS:HG3	1.64	0.78
1:A:140:VAL:O	1:A:143:LEU:HD12	1.83	0.78
1:B:133:LEU:HB3	1:B:134:PRO:HD3	1.66	0.77
1:A:173:ASP:HA	1:A:176:HIS:HB2	1.66	0.77
1:B:241:LEU:O	1:B:241:LEU:HD23	1.84	0.77
1:A:171:VAL:HA	1:A:174:MET:SD	2.24	0.77
1:B:-1:ARG:O	1:B:-1:ARG:HG2	1.85	0.76
1:B:162:ILE:HD11	1:B:171:VAL:HG21	1.65	0.76
1:A:192:SER:OG	1:A:200:ILE:HD11	1.85	0.76
1:B:91:LEU:O	1:B:91:LEU:HD12	1.84	0.76
1:B:124:GLY:HA3	1:B:152:PHE:CE2	2.21	0.76
1:B:207:ARG:NE	1:B:250:ASN:HD22	1.84	0.75
1:A:-5:HIS:O	1:A:-2:VAL:HG23	1.86	0.75
1:A:108:LEU:HG	1:A:109:VAL:N	2.01	0.75
1:A:28:LEU:CB	1:A:35:ILE:HD11	2.17	0.75
1:A:197:ASN:C	1:A:198:TYR:HD2	1.90	0.75
1:A:214:VAL:HG23	1:A:214:VAL:O	1.85	0.74
1:A:147:ILE:HD11	1:A:183:VAL:CG2	2.17	0.74
1:A:168:ALA:O	1:A:172:MET:HG3	1.86	0.74
1:A:78:ASP:C	1:A:108:LEU:HD12	2.08	0.74
1:A:230:PHE:CD1	1:A:267:LEU:HD22	2.23	0.74
1:A:147:ILE:HD11	1:A:183:VAL:HA	1.68	0.73
1:A:169:LEU:HD23	1:A:172:MET:HE2	1.69	0.73
1:A:147:ILE:CD1	1:A:183:VAL:HA	2.19	0.73
1:B:296:SER:O	1:B:300:ILE:HG12	1.88	0.73
1:A:93:MET:O	1:A:97:ILE:HG13	1.88	0.73
1:A:199:LEU:CB	1:A:223:ILE:HB	2.16	0.73
1:B:35:ILE:HD13	1:B:36:ASP:N	2.03	0.73
1:B:151:GLN:HB2	1:B:188:SER:HA	1.71	0.73
1:B:79:TYR:OH	1:B:246:HIS:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:HA2	1:B:71:LEU:HD12	1.70	0.73
1:B:206:ARG:HG3	1:B:207:ARG:N	2.03	0.73
1:A:135:VAL:HG13	1:A:139:LYS:HD2	1.69	0.73
1:A:28:LEU:O	1:A:33:PHE:HB2	1.88	0.73
1:A:12:SER:HB2	1:A:41:VAL:HG22	1.71	0.73
1:A:152:PHE:CZ	1:A:156:LEU:HG	2.23	0.73
1:A:244:TRP:CE3	1:A:258:LYS:HD2	2.24	0.72
1:B:112:CYS:O	1:B:147:ILE:HA	1.89	0.72
1:A:186:THR:HA	1:A:201:VAL:CG1	2.20	0.72
1:B:1:MET:O	1:B:1:MET:HG2	1.88	0.72
1:A:72:ASN:HD21	1:A:74:MET:CG	2.02	0.71
1:A:42:GLN:HE22	1:B:39:ASN:H	1.35	0.71
1:A:193:PRO:HD3	1:A:220:ARG:HH12	1.56	0.71
1:A:4:GLU:HG2	1:A:6:ARG:NH2	2.06	0.71
1:B:278:ALA:O	1:B:279:GLY:O	2.08	0.71
1:B:265:HIS:HD2	1:B:303:PRO:HB3	1.56	0.71
1:B:115:VAL:CG2	1:B:115:VAL:O	2.39	0.71
1:B:95:VAL:HG12	1:B:96:ASP:N	2.03	0.71
1:B:26:PHE:HB3	1:B:27:PRO:HD3	1.71	0.71
1:A:200:ILE:HD12	1:A:220:ARG:HD3	1.73	0.70
1:A:78:ASP:O	1:A:108:LEU:HD12	1.91	0.70
1:A:254:VAL:CA	1:A:257:GLU:HB2	2.21	0.70
1:B:311:VAL:O	1:B:312:LEU:HD23	1.91	0.70
1:A:72:ASN:OD1	1:A:74:MET:HB2	1.92	0.69
1:A:271:ILE:HD13	1:A:274:ALA:HB3	1.74	0.69
1:B:162:ILE:HD11	1:B:171:VAL:HG23	1.73	0.69
1:A:35:ILE:HD12	1:A:35:ILE:N	2.04	0.69
1:A:198:TYR:HA	1:A:223:ILE:O	1.93	0.69
1:A:128:VAL:HG13	1:A:132:LEU:HD13	1.73	0.69
1:A:29:GLN:O	1:B:294:VAL:HG13	1.92	0.69
1:B:239:ALA:O	1:B:242:LEU:HB3	1.92	0.69
1:B:200:ILE:HG22	1:B:201:VAL:H	1.58	0.69
1:B:172:MET:HA	1:B:175:LEU:HD12	1.72	0.69
1:A:27:PRO:HG3	1:A:300:ILE:HD13	1.76	0.68
1:B:115:VAL:CG1	1:B:136:TYR:HE1	2.07	0.68
1:B:141:VAL:HG21	1:B:157:LEU:HD22	1.75	0.68
1:A:186:THR:HA	1:A:201:VAL:HG13	1.74	0.68
1:B:273:CYS:SG	1:B:292:ARG:HG3	2.34	0.68
1:B:120:TRP:HE3	1:B:120:TRP:C	1.97	0.68
1:B:5:CYS:HA	1:B:78:ASP:OD2	1.93	0.68
1:A:264:HIS:CD2	1:A:268:GLN:HG3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:HG3	1:B:220:ARG:HH11	1.56	0.68
1:B:190:LEU:HD13	1:B:200:ILE:HG13	1.76	0.68
1:B:66:TYR:HA	1:B:69:LEU:HD12	1.76	0.68
1:B:197:ASN:HA	1:B:225:LYS:HD2	1.75	0.67
1:B:260:VAL:HA	1:B:263:LEU:HD23	1.74	0.67
1:B:115:VAL:HG22	1:B:115:VAL:O	1.93	0.67
1:A:36:ASP:HA	1:B:22:ARG:HH12	1.59	0.67
1:A:236:LEU:O	1:A:236:LEU:HD12	1.95	0.67
1:A:218:ARG:O	1:A:219:ILE:HG23	1.95	0.67
1:B:197:ASN:O	1:B:225:LYS:HB3	1.95	0.67
1:B:80:VAL:HG23	1:B:108:LEU:HD21	1.77	0.67
1:A:56:VAL:HG12	1:A:57:LEU:O	1.94	0.67
1:A:15:ILE:O	1:A:15:ILE:HG22	1.95	0.67
1:A:62:LEU:HD22	1:A:90:PHE:CZ	2.29	0.67
1:A:193:PRO:HD3	1:A:220:ARG:NH1	2.09	0.67
1:B:172:MET:HE2	1:B:185:ILE:HG13	1.77	0.67
1:A:4:GLU:HG2	1:A:6:ARG:CZ	2.25	0.66
1:A:39:ASN:H	1:B:42:GLN:HE22	1.42	0.66
1:A:162:ILE:HG21	1:A:168:ALA:HB2	1.77	0.66
1:A:172:MET:O	1:A:175:LEU:HB2	1.94	0.66
1:A:16:ARG:HD2	1:B:74:MET:HB3	1.76	0.66
1:A:28:LEU:HD22	1:A:33:PHE:CD1	2.30	0.66
1:A:155:GLU:CG	1:A:162:ILE:HG12	2.26	0.66
1:B:223:ILE:HD13	1:B:223:ILE:N	2.11	0.66
1:A:199:LEU:HB2	1:A:223:ILE:CB	2.20	0.65
1:B:205:GLN:HB3	1:B:252:LEU:HD11	1.79	0.65
1:A:15:ILE:HD12	1:A:43:PHE:O	1.97	0.65
1:B:12:SER:HB2	1:B:41:VAL:HG22	1.79	0.65
1:B:127:TYR:O	1:B:128:VAL:HG13	1.97	0.65
1:A:88:LYS:HG3	1:A:135:VAL:HG21	1.78	0.65
1:A:94:VAL:O	1:A:98:VAL:HG23	1.97	0.65
1:B:-8:HIS:NE2	1:B:-7:HIS:CE1	2.64	0.65
1:A:151:GLN:HB2	1:A:188:SER:HA	1.79	0.65
1:A:153:GLU:O	1:A:157:LEU:HD12	1.97	0.65
1:A:147:ILE:HD12	1:A:180:PRO:CB	2.27	0.64
1:B:142:PRO:HA	1:B:178:MET:O	1.97	0.64
1:B:120:TRP:CE3	1:B:120:TRP:C	2.70	0.64
1:B:242:LEU:C	1:B:242:LEU:HD23	2.18	0.64
1:B:115:VAL:CG1	1:B:136:TYR:CE1	2.80	0.64
1:A:45:ASN:HD21	1:B:72:ASN:HD22	1.45	0.64
1:B:7:VAL:HB	1:B:35:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:VAL:C	1:B:312:LEU:HD23	2.18	0.64
1:A:147:ILE:HD11	1:A:183:VAL:HG22	1.78	0.64
1:A:209:ASN:HB2	1:A:210:PRO:HD2	1.79	0.64
1:A:79:TYR:CD2	1:A:109:VAL:HB	2.33	0.64
1:B:265:HIS:CD2	1:B:303:PRO:HB3	2.33	0.63
1:B:252:LEU:HB3	1:B:256:CYS:SG	2.39	0.63
1:A:147:ILE:CD1	1:A:180:PRO:HB3	2.27	0.63
1:B:202:LEU:HD23	1:B:203:GLY:N	2.13	0.63
1:B:280:GLU:O	1:B:280:GLU:HG3	1.98	0.63
1:B:206:ARG:HD2	1:B:208:ARG:HD3	1.81	0.63
1:B:136:TYR:CE2	1:B:140:VAL:HG11	2.34	0.63
1:B:223:ILE:HG22	1:B:307:VAL:HG11	1.80	0.63
1:A:155:GLU:HG3	1:A:162:ILE:HG12	1.80	0.62
1:A:230:PHE:HE1	1:A:267:LEU:CB	2.09	0.62
1:B:172:MET:CE	1:B:202:LEU:HD22	2.29	0.62
1:A:91:LEU:HA	1:A:94:VAL:HG23	1.80	0.62
1:B:13:HIS:O	1:B:42:GLN:HA	2.00	0.62
1:A:268:GLN:O	1:A:272:GLN:HB2	1.99	0.62
1:A:28:LEU:HB3	1:A:35:ILE:HD11	1.82	0.62
1:B:133:LEU:HD21	1:B:137:LYS:HE3	1.81	0.61
1:A:38:VAL:HA	1:B:15:ILE:HD12	1.82	0.61
1:B:250:ASN:N	1:B:250:ASN:OD1	2.32	0.61
1:A:168:ALA:O	1:A:171:VAL:HG12	1.99	0.61
1:B:214:VAL:HG22	1:B:215:VAL:N	2.15	0.61
1:A:119:LYS:HG2	1:A:123:GLU:O	2.00	0.61
1:A:6:ARG:O	1:A:7:VAL:HG23	2.00	0.61
1:A:229:VAL:HG12	1:A:229:VAL:O	2.00	0.61
1:B:205:GLN:HB2	1:B:252:LEU:HD11	1.81	0.61
1:A:254:VAL:HA	1:A:257:GLU:CB	2.29	0.61
1:A:28:LEU:HD22	1:A:33:PHE:HD1	1.65	0.60
1:A:47:THR:HG22	1:A:52:TRP:CE2	2.36	0.60
1:B:118:ASP:CG	1:B:119:LYS:H	2.05	0.60
1:A:16:ARG:HH11	1:B:74:MET:HG2	1.64	0.60
1:B:8:LEU:HD13	1:B:77:TYR:CZ	2.36	0.60
1:B:26:PHE:HD1	1:B:26:PHE:C	2.03	0.60
1:A:28:LEU:C	1:A:35:ILE:HD11	2.21	0.60
1:B:115:VAL:CG2	1:B:128:VAL:HG11	2.31	0.60
1:A:12:SER:HB2	1:A:41:VAL:CG2	2.30	0.60
1:B:274:ALA:HA	1:B:288:GLN:O	2.01	0.60
1:B:133:LEU:CG	1:B:137:LYS:HE3	2.32	0.59
1:B:262:THR:O	1:B:266:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:CE1	1:B:286:PRO:HB2	2.37	0.59
1:A:252:LEU:HD11	1:A:256:CYS:SG	2.42	0.59
1:B:198:TYR:HE1	1:B:224:ARG:HE	1.48	0.59
1:A:171:VAL:HG13	1:A:172:MET:N	2.18	0.59
1:A:206:ARG:HG3	1:A:216:MET:HG3	1.85	0.59
1:B:26:PHE:CD1	1:B:26:PHE:C	2.76	0.59
1:A:147:ILE:HD13	1:A:147:ILE:N	1.96	0.59
1:A:220:ARG:HG3	1:A:221:MET:N	2.18	0.58
1:B:84:TYR:CD2	1:B:115:VAL:HG23	2.38	0.58
1:B:-5:HIS:O	1:B:-2:VAL:HG23	2.03	0.58
1:A:136:TYR:HA	1:A:140:VAL:HB	1.85	0.58
1:A:264:HIS:HD2	1:A:268:GLN:HG3	1.67	0.58
1:B:208:ARG:HA	1:B:214:VAL:HA	1.84	0.58
1:B:70:ARG:HG3	1:B:75:ASN:ND2	2.18	0.58
1:A:261:SER:O	1:A:264:HIS:HB3	2.03	0.58
1:B:133:LEU:CD2	1:B:137:LYS:HE3	2.34	0.58
1:A:254:VAL:HG12	1:A:258:LYS:CG	2.30	0.58
1:B:98:VAL:HG11	1:B:110:TYR:CD1	2.39	0.58
1:B:57:LEU:HD11	1:B:65:LEU:HD22	1.86	0.57
1:B:0:THR:HG22	1:B:1:MET:N	2.19	0.57
1:A:45:ASN:HD22	1:B:74:MET:CE	2.18	0.57
1:B:69:LEU:HD23	1:B:74:MET:CE	2.35	0.57
1:B:214:VAL:HG22	1:B:215:VAL:O	2.04	0.57
1:A:53:LYS:HG2	1:B:64:GLU:OE1	2.05	0.57
1:A:242:LEU:C	1:A:242:LEU:HD23	2.25	0.57
1:A:181:ASP:HB2	1:A:207:ARG:CZ	2.35	0.57
1:A:197:ASN:O	1:A:225:LYS:HD3	2.04	0.57
1:A:26:PHE:HB3	1:A:27:PRO:CD	2.28	0.57
1:B:176:HIS:HD1	1:B:181:ASP:HA	1.70	0.57
1:A:151:GLN:CB	1:A:188:SER:HA	2.34	0.56
1:A:169:LEU:HD23	1:A:172:MET:CE	2.33	0.56
1:B:84:TYR:HD2	1:B:115:VAL:HG23	1.70	0.56
1:B:115:VAL:HG22	1:B:128:VAL:HG11	1.88	0.56
1:A:4:GLU:HB3	1:A:6:ARG:CG	2.32	0.56
1:B:210:PRO:HG2	1:B:215:VAL:HG13	1.88	0.56
1:B:287:MET:N	1:B:287:MET:SD	2.70	0.56
1:A:139:LYS:O	1:A:143:LEU:HD11	2.06	0.56
1:B:91:LEU:HD11	1:B:140:VAL:CG2	2.35	0.56
1:A:186:THR:CA	1:A:201:VAL:HG13	2.35	0.56
1:B:14:VAL:HA	1:B:43:PHE:O	2.05	0.56
1:B:128:VAL:HB	1:B:132:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:HD21	1:B:72:ASN:ND2	2.02	0.56
1:A:45:ASN:HD22	1:B:74:MET:HE1	1.71	0.56
1:B:57:LEU:CD2	1:B:62:LEU:HB2	2.36	0.56
1:A:165:GLN:HG3	1:A:166:GLU:N	2.20	0.55
1:A:12:SER:CB	1:A:41:VAL:HG22	2.36	0.55
1:A:153:GLU:O	1:A:157:LEU:HB2	2.06	0.55
1:B:120:TRP:HE3	1:B:120:TRP:O	1.87	0.55
1:A:16:ARG:NH1	1:B:74:MET:HG2	2.21	0.55
1:B:97:ILE:O	1:B:101:LEU:HG	2.06	0.55
1:B:133:LEU:HG	1:B:137:LYS:HE3	1.88	0.55
1:B:115:VAL:HG12	1:B:136:TYR:CE1	2.42	0.54
1:A:257:GLU:OE1	1:A:305:ILE:HD12	2.08	0.54
1:A:18:TYR:HD2	1:A:293:MET:HG3	1.72	0.54
1:B:26:PHE:CE2	1:B:294:VAL:HA	2.42	0.54
1:A:311:VAL:HG12	1:A:312:LEU:N	2.23	0.54
1:A:160:ARG:HG3	1:A:160:ARG:HH11	1.73	0.54
1:B:71:LEU:C	1:B:73:ASN:H	2.11	0.54
1:A:241:LEU:O	1:A:245:THR:HG23	2.07	0.54
1:A:220:ARG:O	1:A:221:MET:HG3	2.07	0.54
1:B:165:GLN:CG	1:B:220:ARG:NH1	2.69	0.54
1:A:45:ASN:ND2	1:B:72:ASN:HD22	2.05	0.54
1:B:273:CYS:HB2	1:B:292:ARG:NH2	2.23	0.54
1:A:270:THR:HA	1:A:292:ARG:HD2	1.90	0.54
1:B:162:ILE:HD12	1:B:167:GLU:C	2.28	0.54
1:B:46:HIS:CE1	1:B:48:GLY:HA3	2.42	0.54
1:A:248:HIS:N	1:A:248:HIS:CD2	2.75	0.54
1:B:0:THR:HG22	1:B:1:MET:H	1.72	0.54
1:A:256:CYS:O	1:A:260:VAL:HG23	2.08	0.54
1:A:18:TYR:N	1:A:18:TYR:CD1	2.75	0.54
1:A:32:GLY:HA2	1:B:294:VAL:HG11	1.89	0.53
1:A:6:ARG:CZ	1:B:16:ARG:HH21	2.22	0.53
1:B:147:ILE:HB	1:B:149:PRO:HD3	1.90	0.53
1:A:254:VAL:C	1:A:257:GLU:HB2	2.28	0.53
1:B:225:LYS:HG3	1:B:225:LYS:O	2.09	0.53
1:A:242:LEU:O	1:A:242:LEU:HD23	2.07	0.53
1:B:130:GLU:HG2	1:B:130:GLU:O	2.09	0.53
1:A:155:GLU:OE2	1:A:162:ILE:HG12	2.08	0.53
1:A:186:THR:HG23	1:A:237:PHE:CE1	2.44	0.53
1:B:67:GLU:O	1:B:68:GLY:C	2.46	0.53
1:A:16:ARG:HH11	1:B:74:MET:CG	2.22	0.53
1:B:200:ILE:HD13	1:B:200:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:O	1:B:223:ILE:HD13	2.09	0.53
1:B:115:VAL:HG13	1:B:136:TYR:HE1	1.73	0.53
1:B:189:ASP:O	1:B:191:PRO:CD	2.48	0.53
1:A:248:HIS:N	1:A:249:PRO:CD	2.72	0.53
1:A:237:PHE:HD1	1:A:263:LEU:HD12	1.74	0.53
1:A:165:GLN:HA	1:A:190:LEU:HD13	1.90	0.52
1:B:137:LYS:O	1:B:142:PRO:HD3	2.09	0.52
1:A:181:ASP:CB	1:A:207:ARG:NH2	2.67	0.52
1:B:217:GLU:OE2	1:B:219:ILE:HG23	2.08	0.52
1:A:208:ARG:HG2	1:A:213:SER:C	2.30	0.52
1:A:118:ASP:CB	1:A:127:TYR:OH	2.57	0.52
1:B:115:VAL:HG12	1:B:136:TYR:OH	2.09	0.52
1:A:28:LEU:HB2	1:A:35:ILE:HD11	1.91	0.52
1:A:32:GLY:HA2	1:B:294:VAL:CG1	2.40	0.52
1:A:244:TRP:C	1:A:246:HIS:H	2.13	0.52
1:B:-10:HIS:C	1:B:-8:HIS:H	2.12	0.52
1:B:28:LEU:O	1:B:33:PHE:HB2	2.10	0.52
1:B:9:SER:CB	1:B:35:ILE:HD11	2.40	0.52
1:A:19:VAL:HG12	1:A:231:VAL:HG12	1.91	0.52
1:A:247:LYS:HG3	1:A:247:LYS:O	2.08	0.52
1:B:172:MET:HE3	1:B:185:ILE:HD12	1.92	0.52
1:A:311:VAL:HG12	1:A:312:LEU:H	1.75	0.52
1:A:35:ILE:H	1:A:35:ILE:CD1	2.10	0.51
1:A:8:LEU:HB2	1:A:77:TYR:CD2	2.44	0.51
1:A:292:ARG:HG2	1:A:292:ARG:NH1	2.24	0.51
1:A:147:ILE:H	1:A:147:ILE:HD12	1.69	0.51
1:A:15:ILE:O	1:A:15:ILE:CG2	2.58	0.51
1:B:188:SER:HB2	1:B:190:LEU:HD12	1.91	0.51
1:A:305:ILE:HG12	1:A:305:ILE:O	2.10	0.51
1:B:220:ARG:C	1:B:221:MET:HG3	2.30	0.51
1:A:114:PRO:O	1:A:116:LEU:HG	2.10	0.51
1:A:44:SER:OG	1:A:45:ASN:ND2	2.43	0.51
1:A:162:ILE:CG2	1:A:168:ALA:HB2	2.39	0.51
1:A:148:THR:N	1:A:149:PRO:CD	2.74	0.51
1:B:114:PRO:HG2	1:B:157:LEU:HD11	1.92	0.51
1:B:162:ILE:HD12	1:B:167:GLU:HB3	1.93	0.51
1:B:188:SER:HB2	1:B:190:LEU:CD1	2.40	0.51
1:B:120:TRP:CE3	1:B:121:ASP:N	2.79	0.51
1:B:12:SER:HB2	1:B:41:VAL:CG2	2.41	0.51
1:B:133:LEU:HB3	1:B:134:PRO:CD	2.39	0.51
1:B:124:GLY:CA	1:B:152:PHE:CE2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:HA	1:A:301:GLU:OE2	2.10	0.51
1:A:108:LEU:O	1:A:109:VAL:CG2	2.58	0.51
1:B:225:LYS:O	1:B:227:ASP:N	2.44	0.51
1:A:185:ILE:HG22	1:A:185:ILE:O	2.11	0.51
1:B:98:VAL:HG12	1:B:143:LEU:HD13	1.92	0.51
1:B:148:THR:N	1:B:149:PRO:HD3	2.25	0.51
1:B:206:ARG:HD3	1:B:214:VAL:HG21	1.93	0.51
1:B:30:VAL:O	1:B:30:VAL:HG22	2.11	0.50
1:A:118:ASP:HB3	1:A:127:TYR:OH	2.11	0.50
1:A:108:LEU:CG	1:A:109:VAL:H	2.17	0.50
1:B:124:GLY:HA3	1:B:152:PHE:HE2	1.71	0.50
1:A:152:PHE:O	1:A:155:GLU:N	2.44	0.50
1:A:36:ASP:OD1	1:B:16:ARG:HD3	2.10	0.50
1:B:206:ARG:NH1	1:B:206:ARG:HB2	2.26	0.50
1:A:18:TYR:N	1:A:18:TYR:HD1	2.10	0.50
1:A:194:GLN:O	1:A:195:GLY:O	2.30	0.50
1:B:115:VAL:HG13	1:B:136:TYR:CE1	2.47	0.50
1:A:75:ASN:O	1:A:101:LEU:CD2	2.60	0.50
1:A:135:VAL:O	1:A:139:LYS:HB2	2.12	0.50
1:A:277:GLN:C	1:A:288:GLN:HE22	2.14	0.50
1:B:116:LEU:HD12	1:B:126:MET:CE	2.41	0.50
1:A:246:HIS:C	1:A:249:PRO:HD3	2.32	0.50
1:A:90:PHE:O	1:A:93:MET:HB3	2.11	0.50
1:A:71:LEU:HB3	1:B:51:HIS:CD2	2.46	0.50
1:A:192:SER:O	1:A:193:PRO:C	2.47	0.50
1:B:220:ARG:HG2	1:B:221:MET:N	2.27	0.50
1:A:139:LYS:O	1:A:143:LEU:CD1	2.60	0.50
1:B:223:ILE:HD13	1:B:223:ILE:H	1.75	0.50
1:A:192:SER:C	1:A:194:GLN:N	2.63	0.50
1:B:223:ILE:O	1:B:224:ARG:C	2.46	0.50
1:A:51:HIS:HB2	1:B:72:ASN:OD1	2.11	0.50
1:B:91:LEU:HD11	1:B:140:VAL:HG21	1.93	0.49
1:B:210:PRO:HG2	1:B:215:VAL:HG11	1.91	0.49
1:A:111:VAL:HG22	1:A:146:ILE:HB	1.92	0.49
1:B:157:LEU:HB2	1:B:175:LEU:HD21	1.94	0.49
1:A:203:GLY:HA3	1:A:219:ILE:HD11	1.94	0.49
1:B:209:ASN:CG	1:B:210:PRO:HD3	2.33	0.49
1:A:26:PHE:CB	1:A:27:PRO:HD3	2.31	0.49
1:B:257:GLU:O	1:B:261:SER:HB2	2.12	0.49
1:A:209:ASN:O	1:A:210:PRO:C	2.51	0.49
1:A:253:LYS:O	1:A:257:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:C	1:B:194:GLN:H	2.16	0.49
1:B:80:VAL:CG2	1:B:108:LEU:HD21	2.42	0.49
1:B:58:ASN:OD1	1:B:61:GLU:N	2.43	0.49
1:A:180:PRO:C	1:A:182:THR:H	2.15	0.49
1:A:273:CYS:C	1:A:275:LYS:N	2.64	0.49
1:B:207:ARG:HE	1:B:250:ASN:HD22	1.59	0.49
1:B:182:THR:OG1	1:B:205:GLN:NE2	2.44	0.49
1:A:148:THR:N	1:A:149:PRO:HD2	2.28	0.49
1:A:254:VAL:HG12	1:A:254:VAL:O	2.12	0.49
1:A:284:PRO:CB	1:A:289:LEU:HG	2.43	0.49
1:B:268:GLN:O	1:B:271:ILE:HG22	2.13	0.49
1:A:43:PHE:HA	1:A:54:GLY:HA3	1.94	0.48
1:B:66:TYR:CD2	1:B:97:ILE:HG13	2.48	0.48
1:A:79:TYR:OH	1:A:246:HIS:ND1	2.42	0.48
1:A:247:LYS:HB3	1:A:248:HIS:CD2	2.48	0.48
1:B:192:SER:O	1:B:194:GLN:N	2.46	0.48
1:B:271:ILE:HG23	1:B:272:GLN:N	2.29	0.48
1:A:51:HIS:CD2	1:B:71:LEU:HB3	2.48	0.48
1:B:82:THR:HB	1:B:110:TYR:HE2	1.78	0.48
1:A:269:ARG:NH1	1:A:299:ASP:OD1	2.44	0.48
1:B:197:ASN:O	1:B:199:LEU:HD12	2.13	0.48
1:A:171:VAL:CG1	1:A:172:MET:N	2.77	0.48
1:A:58:ASN:O	1:A:59:SER:C	2.51	0.48
1:B:185:ILE:O	1:B:187:SER:N	2.46	0.48
1:A:268:GLN:O	1:A:272:GLN:N	2.46	0.48
1:A:-2:VAL:HG12	1:A:-2:VAL:O	2.12	0.48
1:A:72:ASN:ND2	1:A:74:MET:CG	2.67	0.48
1:B:279:GLY:C	1:B:281:GLY:H	2.17	0.48
1:A:17:GLY:C	1:A:18:TYR:HD1	2.17	0.48
1:A:70:ARG:O	1:A:73:ASN:N	2.43	0.48
1:A:74:MET:HE1	2:B:363:HOH:O	2.13	0.48
1:B:162:ILE:HD12	1:B:167:GLU:O	2.14	0.48
1:B:9:SER:HB3	1:B:35:ILE:HD11	1.96	0.48
1:B:165:GLN:CG	1:B:220:ARG:HH11	2.24	0.48
1:A:193:PRO:CD	1:A:220:ARG:NH1	2.77	0.48
1:A:268:GLN:O	1:A:272:GLN:CB	2.61	0.48
1:A:102:LYS:C	1:A:104:GLN:N	2.67	0.48
1:A:252:LEU:CD1	1:A:256:CYS:SG	3.02	0.48
1:A:207:ARG:O	1:A:215:VAL:HG13	2.13	0.48
1:B:192:SER:HB2	1:B:200:ILE:HD12	1.94	0.48
1:B:152:PHE:O	1:B:156:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:THR:C	1:A:201:VAL:HG13	2.33	0.47
1:B:192:SER:HB2	1:B:220:ARG:HH21	1.79	0.47
1:A:124:GLY:O	1:A:125:SER:HB2	2.14	0.47
1:A:-10:HIS:C	1:A:-8:HIS:H	2.17	0.47
1:B:25:THR:HG23	1:B:35:ILE:HG21	1.96	0.47
1:A:62:LEU:HD23	1:A:93:MET:HB3	1.95	0.47
1:B:150:ASN:C	1:B:150:ASN:OD1	2.52	0.47
1:A:190:LEU:CD1	1:A:202:LEU:HD11	2.44	0.47
1:A:28:LEU:HB2	1:A:35:ILE:CD1	2.44	0.47
1:A:252:LEU:O	1:A:252:LEU:HG	2.13	0.47
1:B:80:VAL:HG11	1:B:98:VAL:HG22	1.96	0.47
1:A:165:GLN:OE1	1:A:220:ARG:NH2	2.48	0.47
1:A:165:GLN:O	1:A:168:ALA:HB3	2.14	0.47
1:B:136:TYR:O	1:B:141:VAL:HG23	2.14	0.47
1:A:269:ARG:NH2	1:A:299:ASP:OD1	2.46	0.47
1:A:102:LYS:NZ	1:A:143:LEU:O	2.47	0.47
1:A:17:GLY:C	1:A:18:TYR:CD1	2.88	0.47
1:A:133:LEU:O	1:A:137:LYS:HD3	2.15	0.47
1:A:147:ILE:HD13	1:A:183:VAL:HA	1.94	0.47
1:B:190:LEU:HD12	1:B:190:LEU:N	2.30	0.47
1:A:102:LYS:HZ2	1:A:143:LEU:HB3	1.79	0.47
1:B:240:MET:HA	1:B:240:MET:CE	2.45	0.47
1:B:269:ARG:O	1:B:269:ARG:HG2	2.15	0.47
1:A:244:TRP:O	1:A:246:HIS:N	2.47	0.47
1:A:95:VAL:HG13	1:A:143:LEU:HD13	1.97	0.47
1:A:60:ASP:HA	1:A:63:GLN:HB3	1.97	0.47
1:A:18:TYR:HD2	1:A:293:MET:CG	2.28	0.47
1:A:57:LEU:HD12	1:A:61:GLU:HB3	1.96	0.47
1:B:165:GLN:OE1	1:B:165:GLN:O	2.32	0.46
1:B:82:THR:CB	1:B:110:TYR:HE2	2.28	0.46
1:A:292:ARG:CG	1:A:292:ARG:HH11	2.28	0.46
1:B:86:ARG:HD2	1:B:129:PRO:HD3	1.97	0.46
1:B:268:GLN:C	1:B:270:THR:H	2.17	0.46
1:B:67:GLU:O	1:B:70:ARG:N	2.49	0.46
1:A:29:GLN:HG3	1:A:35:ILE:HD13	1.97	0.46
1:A:254:VAL:O	1:A:258:LYS:HG3	2.15	0.46
1:A:38:VAL:HG13	1:A:65:LEU:HD12	1.97	0.46
1:B:222:ASP:N	1:B:222:ASP:OD1	2.48	0.46
1:B:57:LEU:HD21	1:B:62:LEU:HB2	1.96	0.46
1:B:285:SER:O	1:B:289:LEU:HB2	2.16	0.46
1:B:79:TYR:OH	1:B:246:HIS:CB	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TYR:CD2	1:A:293:MET:CG	2.98	0.46
1:B:66:TYR:O	1:B:69:LEU:HB2	2.16	0.46
1:B:42:GLN:CG	1:B:42:GLN:O	2.62	0.46
1:A:112:CYS:O	1:A:114:PRO:HD2	2.15	0.46
1:B:252:LEU:HD12	1:B:252:LEU:N	2.31	0.46
1:A:170:ARG:CB	1:A:170:ARG:CZ	2.88	0.46
1:A:133:LEU:HD12	1:A:133:LEU:O	2.15	0.46
1:B:169:LEU:CD2	1:B:202:LEU:HD21	2.45	0.46
1:B:171:VAL:O	1:B:175:LEU:HD12	2.16	0.46
1:A:27:PRO:O	1:A:30:VAL:HG22	2.15	0.46
1:A:240:MET:O	1:A:241:LEU:C	2.53	0.46
1:A:-10:HIS:O	1:A:-8:HIS:N	2.48	0.46
1:A:199:LEU:HD23	1:A:225:LYS:HG2	1.97	0.46
1:A:147:ILE:HD11	1:A:183:VAL:CA	2.41	0.46
1:B:252:LEU:O	1:B:256:CYS:CB	2.64	0.46
1:B:41:VAL:HG12	1:B:56:VAL:HG13	1.98	0.46
1:A:278:ALA:N	1:A:288:GLN:HE22	2.14	0.46
1:B:124:GLY:C	1:B:152:PHE:CE2	2.89	0.46
1:A:42:GLN:OE1	1:B:39:ASN:HB2	2.16	0.46
1:A:223:ILE:HG22	1:A:224:ARG:O	2.16	0.45
1:B:69:LEU:HD23	1:B:74:MET:HE3	1.98	0.45
1:B:282:VAL:HG22	1:B:283:ARG:N	2.31	0.45
1:A:220:ARG:CG	1:A:221:MET:N	2.78	0.45
1:B:283:ARG:O	1:B:283:ARG:HD3	2.16	0.45
1:B:147:ILE:HD11	1:B:183:VAL:HG13	1.98	0.45
1:B:91:LEU:C	1:B:91:LEU:HD12	2.35	0.45
1:B:7:VAL:CB	1:B:35:ILE:HG12	2.46	0.45
1:A:216:MET:SD	1:A:218:ARG:HG3	2.57	0.45
1:B:311:VAL:CG2	2:B:396:HOH:O	2.46	0.45
1:B:199:LEU:C	1:B:200:ILE:HD13	2.36	0.45
1:A:214:VAL:CG2	1:A:214:VAL:O	2.58	0.45
1:B:263:LEU:HD22	1:B:263:LEU:H	1.82	0.45
1:B:297:LYS:O	1:B:298:ARG:C	2.54	0.45
1:B:133:LEU:O	1:B:135:VAL:N	2.48	0.45
1:A:75:ASN:HD21	1:A:104:GLN:HG3	1.81	0.45
1:B:264:HIS:C	1:B:266:VAL:H	2.18	0.45
1:B:29:GLN:C	1:B:31:LEU:H	2.19	0.45
1:A:86:ARG:CG	1:A:86:ARG:O	2.64	0.45
1:B:126:MET:O	1:B:127:TYR:HD2	1.99	0.45
1:A:91:LEU:HA	1:A:94:VAL:CG2	2.46	0.45
1:A:151:GLN:N	1:A:187:SER:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:HG22	1:B:306:VAL:O	2.15	0.45
1:A:198:TYR:CE2	1:A:224:ARG:HD3	2.52	0.45
1:B:116:LEU:HA	1:B:116:LEU:HD13	1.65	0.45
1:B:279:GLY:O	1:B:281:GLY:N	2.49	0.45
1:A:25:THR:O	1:A:26:PHE:C	2.55	0.45
1:A:26:PHE:O	1:A:29:GLN:HB2	2.17	0.45
1:A:244:TRP:C	1:A:246:HIS:N	2.69	0.45
1:A:255:ALA:C	1:A:257:GLU:H	2.20	0.45
1:B:8:LEU:HB2	1:B:77:TYR:CD2	2.51	0.45
1:B:166:GLU:O	1:B:166:GLU:HG2	2.17	0.45
1:A:79:TYR:HH	1:A:246:HIS:CG	2.35	0.45
1:A:284:PRO:HB3	1:A:289:LEU:HG	1.99	0.45
1:B:103:GLN:HB3	1:B:103:GLN:HE21	1.65	0.45
1:B:115:VAL:HG12	1:B:136:TYR:CZ	2.52	0.44
1:B:199:LEU:HD13	1:B:225:LYS:HB3	1.98	0.44
1:B:306:VAL:CG2	1:B:306:VAL:O	2.66	0.44
1:A:103:GLN:O	1:A:103:GLN:NE2	2.50	0.44
1:A:105:ASN:HA	1:A:106:PRO:HD3	1.74	0.44
1:B:166:GLU:OE2	1:B:170:ARG:NH2	2.50	0.44
1:A:28:LEU:HB2	1:A:35:ILE:HG12	1.99	0.44
1:B:62:LEU:HB2	1:B:90:PHE:HE1	1.82	0.44
1:A:273:CYS:O	1:A:276:ALA:N	2.42	0.44
1:B:263:LEU:HD22	1:B:263:LEU:N	2.32	0.44
1:A:53:LYS:HB3	1:B:64:GLU:HG2	1.99	0.44
1:B:160:ARG:CD	1:B:161:LYS:H	2.21	0.44
1:B:167:GLU:HA	1:B:170:ARG:HB2	2.00	0.44
1:A:305:ILE:CG1	1:A:305:ILE:O	2.66	0.44
1:A:5:CYS:SG	1:A:246:HIS:CD2	3.11	0.44
1:A:39:ASN:O	1:A:41:VAL:N	2.50	0.44
1:A:17:GLY:HA3	1:A:290:GLU:OE1	2.17	0.44
1:A:273:CYS:O	1:A:274:ALA:C	2.55	0.44
1:B:5:CYS:HB3	1:B:33:PHE:CD2	2.53	0.44
1:A:47:THR:HA	1:A:52:TRP:CE3	2.52	0.44
1:B:283:ARG:HG2	1:B:283:ARG:HH11	1.81	0.44
1:B:147:ILE:C	1:B:149:PRO:HD3	2.39	0.44
1:A:5:CYS:HG	1:A:246:HIS:CD2	2.36	0.44
1:A:6:ARG:HH11	1:A:6:ARG:HG2	1.83	0.44
1:A:75:ASN:ND2	1:A:104:GLN:HG3	2.32	0.44
1:B:242:LEU:C	1:B:242:LEU:CD2	2.85	0.44
1:B:138:GLU:O	1:B:142:PRO:HG2	2.17	0.44
1:B:16:ARG:NH1	1:B:16:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HE3	1:B:152:PHE:HD2	1.82	0.44
1:B:252:LEU:O	1:B:256:CYS:SG	2.75	0.44
1:A:-2:VAL:O	1:B:272:GLN:NE2	2.51	0.44
1:B:12:SER:CB	1:B:41:VAL:HG22	2.46	0.44
1:A:82:THR:HG21	1:A:94:VAL:HG11	2.00	0.44
1:A:198:TYR:N	1:A:198:TYR:HD2	2.16	0.43
1:A:223:ILE:O	1:A:224:ARG:C	2.56	0.43
1:B:157:LEU:HB2	1:B:175:LEU:CD2	2.48	0.43
1:B:7:VAL:CG1	1:B:35:ILE:HG12	2.49	0.43
1:A:161:LYS:HE3	1:A:161:LYS:HB3	1.66	0.43
1:B:151:GLN:O	1:B:155:GLU:HG3	2.19	0.43
1:B:197:ASN:OD1	1:B:198:TYR:HD1	2.01	0.43
1:B:92:ALA:O	1:B:95:VAL:HB	2.18	0.43
1:B:133:LEU:C	1:B:135:VAL:N	2.72	0.43
1:B:190:LEU:HD13	1:B:200:ILE:CG1	2.48	0.43
1:A:34:GLU:HG2	1:B:18:TYR:OH	2.18	0.43
1:A:147:ILE:HD11	1:A:183:VAL:HG23	1.97	0.43
1:B:40:SER:O	1:B:57:LEU:N	2.47	0.43
1:A:115:VAL:HA	1:A:153:GLU:OE2	2.18	0.43
1:A:242:LEU:C	1:A:242:LEU:CD2	2.87	0.43
1:A:190:LEU:O	1:A:200:ILE:HG13	2.18	0.43
1:B:30:VAL:HG22	1:B:301:GLU:HG2	2.01	0.43
1:A:79:TYR:CE2	1:A:109:VAL:HB	2.53	0.43
1:A:95:VAL:HG13	1:A:143:LEU:CD1	2.49	0.43
1:B:98:VAL:CG1	1:B:143:LEU:HD13	2.48	0.43
1:A:207:ARG:O	1:A:215:VAL:CG1	2.66	0.43
1:A:186:THR:O	1:A:201:VAL:HG13	2.19	0.43
1:A:219:ILE:CD1	1:A:256:CYS:SG	3.07	0.43
1:B:145:ASP:O	1:B:146:ILE:HG13	2.19	0.43
1:B:146:ILE:HG12	1:B:182:THR:HB	2.01	0.43
1:B:270:THR:HA	1:B:292:ARG:HG2	2.01	0.43
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.84	0.43
1:A:130:GLU:HG2	1:A:131:ASP:N	2.33	0.43
1:A:151:GLN:HB2	1:A:188:SER:CA	2.48	0.43
1:A:198:TYR:CD2	1:A:198:TYR:N	2.86	0.43
1:A:113:ASP:O	1:A:115:VAL:N	2.48	0.43
1:B:95:VAL:O	1:B:98:VAL:N	2.52	0.43
1:A:52:TRP:O	1:A:52:TRP:CD1	2.72	0.43
1:A:16:ARG:HG2	1:A:17:GLY:N	2.34	0.42
1:A:15:ILE:O	1:B:36:ASP:HB3	2.20	0.42
1:B:197:ASN:OD1	1:B:198:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-8:HIS:CE1	1:B:-7:HIS:CE1	3.07	0.42
1:B:141:VAL:O	1:B:180:PRO:HD3	2.19	0.42
1:B:176:HIS:ND1	1:B:180:PRO:O	2.52	0.42
1:A:15:ILE:HD11	1:B:65:LEU:HD11	2.01	0.42
1:B:287:MET:HG2	1:B:288:GLN:HG3	2.00	0.42
1:A:140:VAL:HG12	1:A:141:VAL:N	2.33	0.42
1:A:285:SER:OG	1:A:288:GLN:HG3	2.20	0.42
1:B:214:VAL:HG22	1:B:215:VAL:H	1.82	0.42
1:B:252:LEU:O	1:B:256:CYS:HB2	2.19	0.42
1:A:288:GLN:HB3	1:A:288:GLN:HE21	1.60	0.42
1:B:31:LEU:HD11	1:B:240:MET:HE1	2.02	0.42
1:B:162:ILE:CD1	1:B:171:VAL:HG21	2.43	0.42
1:B:27:PRO:HA	1:B:30:VAL:CG1	2.50	0.42
1:B:160:ARG:HD2	1:B:161:LYS:N	2.22	0.42
1:B:205:GLN:OE1	1:B:252:LEU:CD1	2.67	0.42
1:A:273:CYS:SG	1:A:292:ARG:NE	2.90	0.42
1:A:240:MET:SD	1:A:262:THR:HG21	2.59	0.42
1:B:278:ALA:CB	1:B:288:GLN:NE2	2.75	0.42
1:A:248:HIS:CE1	1:A:258:LYS:HE3	2.55	0.42
1:B:285:SER:HB2	1:B:287:MET:SD	2.60	0.42
1:B:268:GLN:O	1:B:270:THR:N	2.52	0.42
1:A:16:ARG:HG2	1:A:17:GLY:H	1.84	0.42
1:A:126:MET:HG2	1:A:128:VAL:H	1.85	0.42
1:B:251:ASN:OD1	1:B:251:ASN:O	2.38	0.42
1:A:171:VAL:O	1:A:175:LEU:HG	2.19	0.42
1:B:1:MET:CG	1:B:1:MET:O	2.64	0.42
1:B:46:HIS:CE1	1:B:48:GLY:CA	3.02	0.42
1:B:192:SER:HB2	1:B:220:ARG:NH2	2.34	0.42
1:B:214:VAL:CG2	1:B:215:VAL:N	2.82	0.42
1:B:74:MET:HE3	1:B:74:MET:HB2	1.78	0.42
1:A:151:GLN:HB2	1:A:188:SER:CB	2.50	0.42
1:B:162:ILE:HG23	1:B:167:GLU:HB2	2.01	0.42
1:B:175:LEU:O	1:B:178:MET:HB2	2.20	0.42
1:A:28:LEU:HD21	1:A:239:ALA:O	2.20	0.42
1:B:25:THR:O	1:B:26:PHE:C	2.58	0.42
1:B:207:ARG:O	1:B:210:PRO:HD2	2.20	0.42
1:A:60:ASP:OD1	1:A:60:ASP:N	2.53	0.42
1:A:294:VAL:C	1:A:296:SER:H	2.23	0.42
1:B:202:LEU:HD23	1:B:203:GLY:H	1.85	0.41
1:A:255:ALA:C	1:A:257:GLU:N	2.74	0.41
1:A:135:VAL:O	1:A:139:LYS:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASN:O	1:A:198:TYR:HD2	2.03	0.41
1:A:230:PHE:CE1	1:A:267:LEU:HD22	2.55	0.41
1:B:257:GLU:O	1:B:261:SER:CB	2.68	0.41
1:B:220:ARG:C	1:B:221:MET:CG	2.88	0.41
1:B:285:SER:OG	1:B:287:MET:SD	2.72	0.41
1:A:17:GLY:CA	1:A:290:GLU:CD	2.89	0.41
1:B:240:MET:HB3	1:B:240:MET:HE2	1.93	0.41
1:A:131:ASP:O	1:A:134:PRO:HD2	2.20	0.41
1:A:218:ARG:O	1:A:219:ILE:CG2	2.68	0.41
1:B:252:LEU:H	1:B:252:LEU:CD1	2.33	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.78	0.41
1:A:209:ASN:CB	1:A:210:PRO:HD2	2.48	0.41
1:A:146:ILE:CG2	1:A:241:LEU:HD23	2.50	0.41
1:A:155:GLU:O	1:A:159:GLY:N	2.43	0.41
1:A:147:ILE:HB	1:A:149:PRO:HD2	2.03	0.41
1:A:235:ASP:O	1:A:239:ALA:HB2	2.20	0.41
1:B:294:VAL:O	1:B:296:SER:N	2.53	0.41
1:B:221:MET:HG2	1:B:309:ALA:HB2	2.03	0.41
1:A:135:VAL:HG13	1:A:139:LYS:HB2	2.03	0.41
1:B:29:GLN:C	1:B:31:LEU:N	2.73	0.41
1:B:6:ARG:HA	1:B:34:GLU:O	2.21	0.41
1:B:26:PHE:HE2	1:B:294:VAL:HA	1.84	0.41
1:A:164:SER:O	1:A:165:GLN:C	2.58	0.41
1:A:252:LEU:HD12	1:A:255:ALA:HB3	2.03	0.41
1:A:116:LEU:HB2	1:A:153:GLU:HG2	2.03	0.41
1:B:230:PHE:CD1	1:B:267:LEU:HD22	2.55	0.41
1:B:175:LEU:HD13	1:B:183:VAL:HG11	2.02	0.41
1:B:206:ARG:HH11	1:B:206:ARG:HB2	1.85	0.41
1:B:118:ASP:CG	1:B:119:LYS:N	2.73	0.41
1:B:80:VAL:HG23	1:B:108:LEU:HD11	2.02	0.41
1:A:197:ASN:C	1:A:198:TYR:CD2	2.81	0.41
1:B:147:ILE:HG12	1:B:180:PRO:HB3	2.03	0.41
1:B:147:ILE:CD1	1:B:183:VAL:HG13	2.51	0.41
1:A:108:LEU:O	1:A:109:VAL:HG22	2.19	0.41
1:A:257:GLU:OE1	1:A:305:ILE:CD1	2.69	0.41
1:B:13:HIS:CE1	1:B:14:VAL:O	2.74	0.41
1:B:252:LEU:HD12	1:B:252:LEU:H	1.86	0.41
1:A:-1:ARG:HE	1:A:-1:ARG:HB2	1.46	0.41
1:A:200:ILE:HD12	1:A:220:ARG:CD	2.48	0.41
1:A:219:ILE:HD11	1:A:252:LEU:HD21	2.02	0.41
1:B:172:MET:HE1	1:B:202:LEU:CD2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:CE2	1:B:241:LEU:HD12	2.56	0.40
1:B:-10:HIS:O	1:B:-10:HIS:CD2	2.74	0.40
1:B:283:ARG:HG2	1:B:283:ARG:NH1	2.36	0.40
1:A:86:ARG:O	1:A:86:ARG:HG3	2.22	0.40
1:A:13:HIS:HB2	1:A:39:ASN:HB3	2.02	0.40
1:B:268:GLN:C	1:B:270:THR:N	2.74	0.40
1:B:273:CYS:SG	1:B:292:ARG:NE	2.94	0.40
1:A:128:VAL:HG11	1:A:132:LEU:HD22	2.02	0.40
1:A:29:GLN:CG	1:A:35:ILE:HD13	2.51	0.40
1:B:274:ALA:CB	1:B:288:GLN:O	2.69	0.40
1:A:28:LEU:HB2	1:A:35:ILE:CG1	2.51	0.40
1:B:210:PRO:O	1:B:211:ALA:C	2.59	0.40
1:A:292:ARG:CG	1:A:292:ARG:NH1	2.83	0.40
1:A:47:THR:HB	1:A:52:TRP:CH2	2.56	0.40
1:A:46:HIS:HE1	1:A:48:GLY:HA3	1.86	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	321/327 (98%)	229 (71%)	65 (20%)	27 (8%)	1	2
1	B	321/327 (98%)	240 (75%)	65 (20%)	16 (5%)	3	8
All	All	642/654 (98%)	469 (73%)	130 (20%)	43 (7%)	1	4

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS
1	A	59	SER
1	A	109	VAL

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Mol	Chain	Res	Type
1	A	195	GLY
1	A	210	PRO
1	A	249	PRO
1	B	186	THR
1	B	279	GLY
1	A	3	GLU
1	A	40	SER
1	A	161	LYS
1	A	214	VAL
1	A	243	ALA
1	A	264	HIS
1	B	228	ALA
1	B	243	ALA
1	B	280	GLU
1	B	295	GLN
1	A	25	THR
1	A	114	PRO
1	A	120	TRP
1	A	245	THR
1	B	193	PRO
1	B	269	ARG
1	A	26	PHE
1	A	69	LEU
1	A	108	LEU
1	A	125	SER
1	A	163	HIS
1	A	180	PRO
1	B	-9	HIS
1	B	253	LYS
1	B	305	ILE
1	A	295	GLN
1	B	259	THR
1	A	122	GLY
1	A	212	GLY
1	B	115	VAL
1	B	249	PRO
1	A	140	VAL
1	B	149	PRO
1	A	115	VAL
1	B	191	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	285/289 (99%)	226 (79%)	59 (21%)	1	4
1	B	285/289 (99%)	223 (78%)	62 (22%)	1	3
All	All	570/578 (99%)	449 (79%)	121 (21%)	1	4

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	1	MET
1	A	18	TYR
1	A	21	ASN
1	A	30	VAL
1	A	46	HIS
1	A	60	ASP
1	A	70	ARG
1	A	72	ASN
1	A	86	ARG
1	A	89	SER
1	A	100	GLU
1	A	103	GLN
1	A	104	GLN
1	A	114	PRO
1	A	121	ASP
1	A	123	GLU
1	A	127	TYR
1	A	130	GLU
1	A	131	ASP
1	A	137	LYS
1	A	142	PRO
1	A	143	LEU
1	A	145	ASP
1	A	147	ILE
1	A	149	PRO
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	157	LEU
1	A	158	SER
1	A	160	ARG
1	A	167	GLU
1	A	170	ARG
1	A	173	ASP
1	A	174	MET
1	A	178	MET
1	A	180	PRO
1	A	191	PRO
1	A	192	SER
1	A	199	LEU
1	A	207	ARG
1	A	210	PRO
1	A	213	SER
1	A	215	VAL
1	A	216	MET
1	A	218	ARG
1	A	221	MET
1	A	226	VAL
1	A	248	HIS
1	A	249	PRO
1	A	256	CYS
1	A	268	GLN
1	A	271	ILE
1	A	272	GLN
1	A	284	PRO
1	A	292	ARG
1	A	302	ASP
1	A	305	ILE
1	A	307	VAL
1	A	308	GLN
1	B	-10	HIS
1	B	-9	HIS
1	B	-8	HIS
1	B	-1	ARG
1	B	0	THR
1	B	1	MET
1	B	2	GLU
1	B	3	GLU
1	B	5	CYS
1	B	21	ASN

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Mol	Chain	Res	Type
1	B	26	PHE
1	B	35	ILE
1	B	45	ASN
1	B	70	ARG
1	B	73	ASN
1	B	91	LEU
1	B	95	VAL
1	B	103	GLN
1	B	106	PRO
1	B	107	ARG
1	B	115	VAL
1	B	116	LEU
1	B	120	TRP
1	B	129	PRO
1	B	134	PRO
1	B	136	TYR
1	B	138	GLU
1	B	143	LEU
1	B	153	GLU
1	B	160	ARG
1	B	165	GLN
1	B	173	ASP
1	B	177	SER
1	B	187	SER
1	B	190	LEU
1	B	191	PRO
1	B	192	SER
1	B	193	PRO
1	B	200	ILE
1	B	206	ARG
1	B	208	ARG
1	B	210	PRO
1	B	215	VAL
1	B	216	MET
1	B	217	GLU
1	B	221	MET
1	B	222	ASP
1	B	223	ILE
1	B	233	THR
1	B	249	PRO
1	B	250	ASN
1	B	260	VAL

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Mol	Chain	Res	Type
1	B	273	CYS
1	B	283	ARG
1	B	284	PRO
1	B	286	PRO
1	B	287	MET
1	B	293	MET
1	B	302	ASP
1	B	304	GLU
1	B	306	VAL
1	B	307	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	21	ASN
1	A	45	ASN
1	A	51	HIS
1	A	55	GLN
1	A	72	ASN
1	A	75	ASN
1	A	103	GLN
1	A	248	HIS
1	A	250	ASN
1	A	251	ASN
1	A	268	GLN
1	A	288	GLN
1	A	308	GLN
1	B	-10	HIS
1	B	-7	HIS
1	B	-5	HIS
1	B	21	ASN
1	B	29	GLN
1	B	42	GLN
1	B	51	HIS
1	B	63	GLN
1	B	73	ASN
1	B	103	GLN
1	B	209	ASN
1	B	248	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	323/327 (98%)	-0.27	0 100 100	36, 44, 50, 56	0
1	B	323/327 (98%)	-0.27	0 100 100	35, 44, 50, 55	0
All	All	646/654 (98%)	-0.27	0 100 100	35, 44, 50, 56	0

There are no RSRZ outliers to report.

### 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.