



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:49 am GMT

PDB ID : 2IQH  
Title : Influenza A virus nucleoprotein NP at 3.2Å resolution  
Authors : Ye, Q.; Tao, Y.J.  
Deposited on : 2006-10-13  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

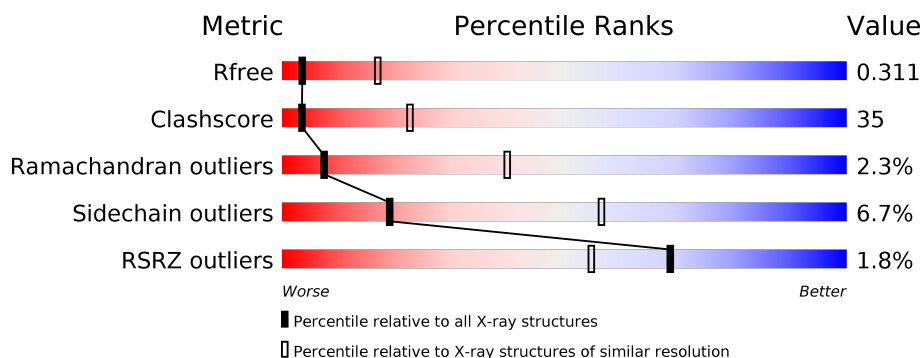
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	499	<div> <div> <div></div> <div>42%</div> <div>38%</div> <div>5%</div> <div>15%</div> </div> </div>
1	B	499	<div> <div> <div></div> <div>44%</div> <div>38%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	499	<div> <div> <div>3%</div> <div>37%</div> <div>44%</div> <div>6%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10162 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 Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	8	0	0
			3358	2084	623	625	26			
1	B	426	Total	C	N	O	S	8	0	0
			3358	2084	623	625	26			
1	C	436	Total	C	N	O	S	8	0	0
			3446	2137	642	641	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	LEU	-	EXPRESSION TAG	UNP Q1I2B5
A	500	GLU	-	EXPRESSION TAG	UNP Q1I2B5
A	501	HIS	-	EXPRESSION TAG	UNP Q1I2B5
A	502	HIS	-	EXPRESSION TAG	UNP Q1I2B5
A	503	HIS	-	EXPRESSION TAG	UNP Q1I2B5
A	504	HIS	-	EXPRESSION TAG	UNP Q1I2B5
A	505	HIS	-	EXPRESSION TAG	UNP Q1I2B5
A	506	HIS	-	EXPRESSION TAG	UNP Q1I2B5
B	499	LEU	-	EXPRESSION TAG	UNP Q1I2B5
B	500	GLU	-	EXPRESSION TAG	UNP Q1I2B5
B	501	HIS	-	EXPRESSION TAG	UNP Q1I2B5
B	502	HIS	-	EXPRESSION TAG	UNP Q1I2B5
B	503	HIS	-	EXPRESSION TAG	UNP Q1I2B5
B	504	HIS	-	EXPRESSION TAG	UNP Q1I2B5
B	505	HIS	-	EXPRESSION TAG	UNP Q1I2B5
B	506	HIS	-	EXPRESSION TAG	UNP Q1I2B5
C	499	LEU	-	EXPRESSION TAG	UNP Q1I2B5
C	500	GLU	-	EXPRESSION TAG	UNP Q1I2B5
C	501	HIS	-	EXPRESSION TAG	UNP Q1I2B5
C	502	HIS	-	EXPRESSION TAG	UNP Q1I2B5
C	503	HIS	-	EXPRESSION TAG	UNP Q1I2B5
C	504	HIS	-	EXPRESSION TAG	UNP Q1I2B5
C	505	HIS	-	EXPRESSION TAG	UNP Q1I2B5

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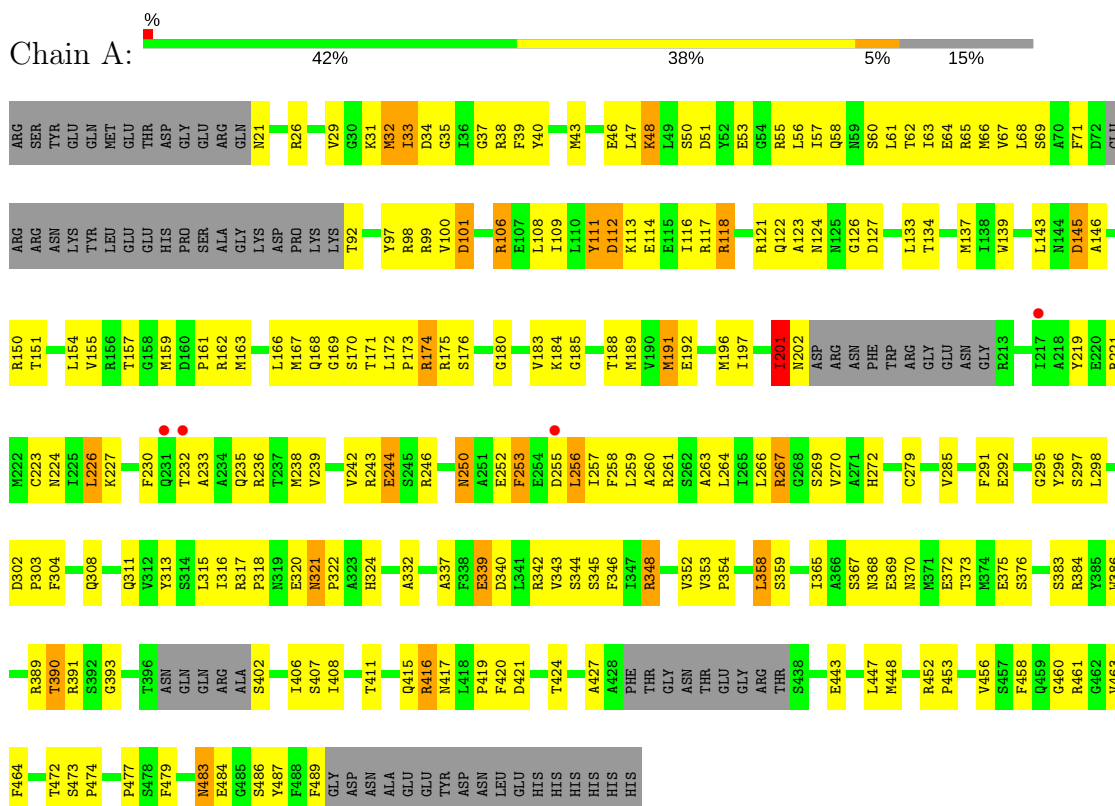
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Chain	Residue	Modelled	Actual	Comment	Reference
C	506	HIS	-	EXPRESSION TAG	UNP Q1I2B5

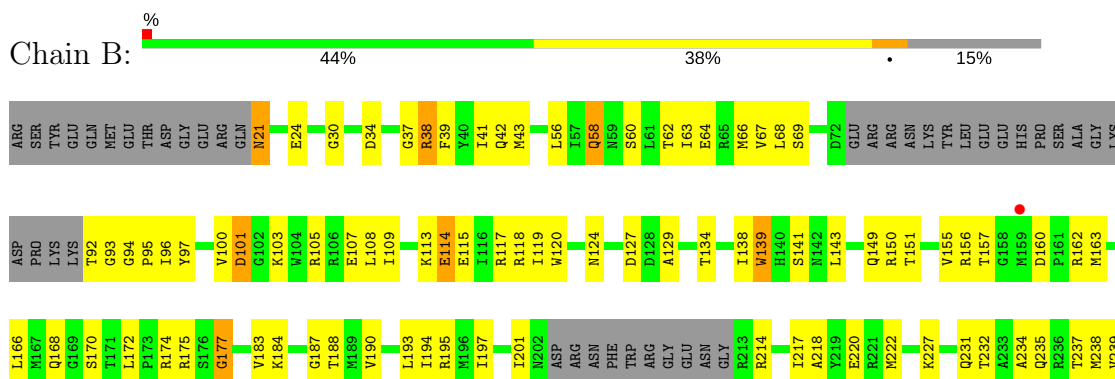
### 3 Residue-property plots

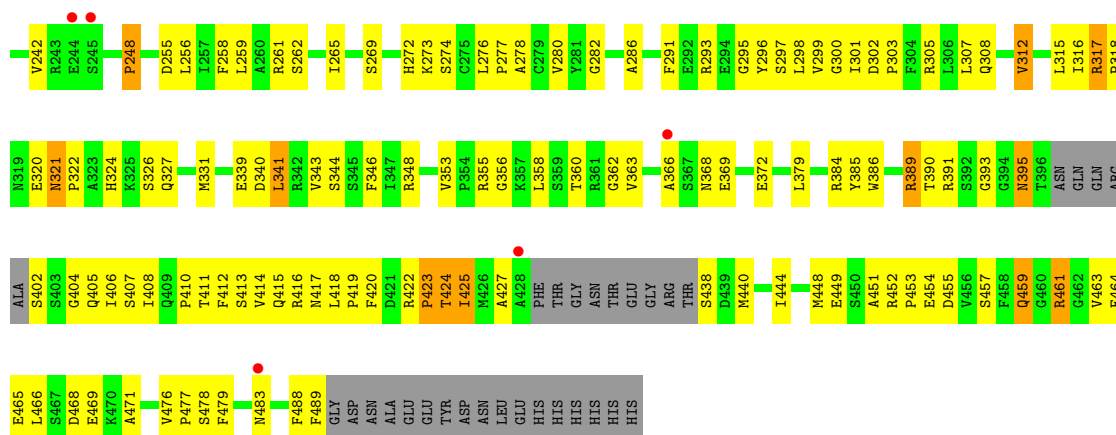
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Nucleocapsid protein

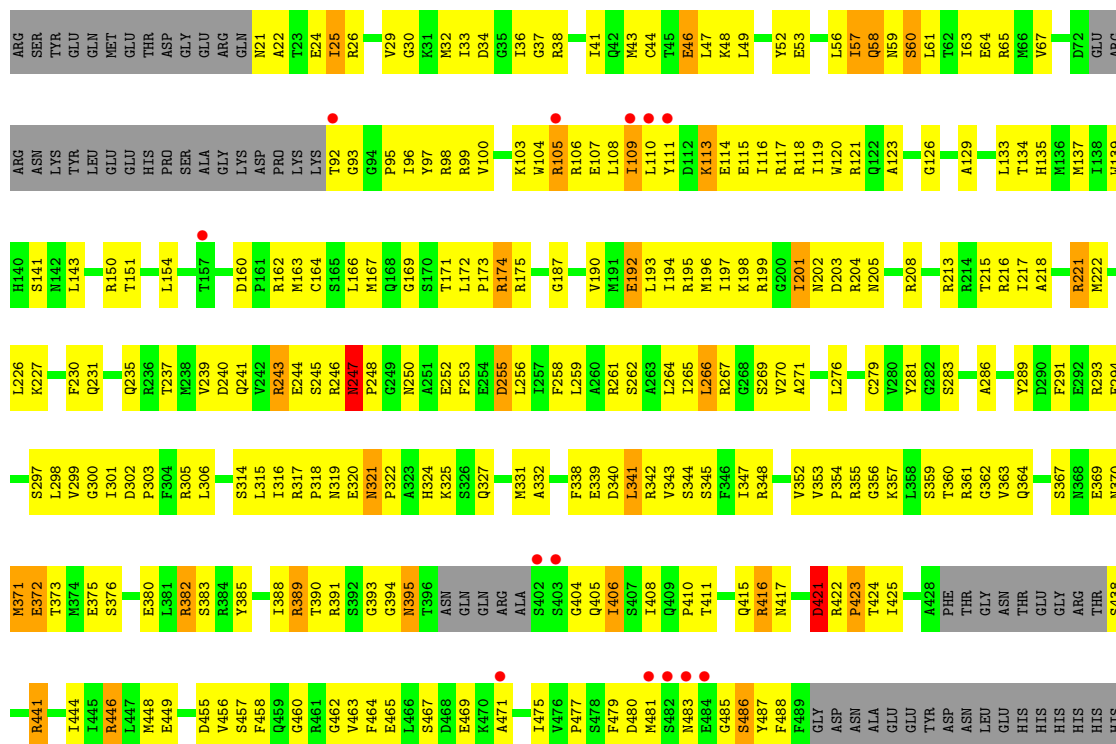


#### • Molecule 1: Nucleocapsid protein





● Molecule 1: Nucleocapsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.10Å 135.10Å 195.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 42.96 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.20) 99.1 (42.96-3.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.271 , 0.318 0.253 , 0.311	Depositor DCC
$R_{free}$ test set	1298 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 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	0.92	1/3411 (0.0%)	0.91	6/4585 (0.1%)
1	B	0.96	3/3411 (0.1%)	0.92	3/4585 (0.1%)
1	C	0.84	4/3503 (0.1%)	0.89	7/4710 (0.1%)
All	All	0.91	8/10325 (0.1%)	0.91	16/13880 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	ILE	C-N	-13.49	1.03	1.34
1	C	201	ILE	C-N	-7.93	1.15	1.34
1	C	202	ASN	C-N	-7.90	1.15	1.34
1	B	312	VAL	CB-CG2	-5.81	1.40	1.52
1	C	247	ASN	CB-CG	5.78	1.64	1.51
1	B	312	VAL	CB-CG1	-5.27	1.41	1.52
1	C	192	GLU	CG-CD	5.26	1.59	1.51
1	A	201	ILE	C-N	-5.25	1.22	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	A	201	ILE	O-C-N	-6.18	112.82	122.70
1	C	221	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	C	201	ILE	O-C-N	-6.15	112.86	122.70
1	B	38	ARG	NE-CZ-NH2	-6.11	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	341	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	A	358	LEU	CB-CG-CD2	-5.70	101.32	111.00
1	A	66	MET	CG-SD-CE	5.51	109.02	100.20
1	B	38	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	256	LEU	CA-CB-CG	5.40	127.72	115.30
1	C	201	ILE	CA-C-N	5.35	128.97	117.20
1	A	145	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	299	VAL	CG1-CB-CG2	-5.31	102.40	110.90
1	A	226	LEU	CA-CB-CG	5.31	127.51	115.30
1	C	421	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	416	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ILE	Mainchain

## 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	3358	0	3355	254	0
1	B	3358	0	3354	222	0
1	C	3446	0	3427	294	0
All	All	10162	0	10136	711	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 35.

All (711) 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:111:TYR:HB3	1:A:116:ILE:HD11	1.46	0.95
1:B:100:VAL:CG2	1:B:105:ARG:HD3	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HG3	1:A:315:LEU:HG	1.50	0.93
1:C:465:GLU:HG3	1:C:467:SER:H	1.32	0.92
1:C:353:VAL:HG22	1:C:354:PRO:HD2	1.52	0.92
1:A:483:ASN:H	1:A:483:ASN:HD22	1.09	0.92
1:A:226:LEU:HD13	1:A:230:PHE:HE1	1.31	0.91
1:C:341:LEU:HB2	1:C:486:SER:HA	1.53	0.90
1:B:21:ASN:CB	1:B:24:GLU:HG3	2.04	0.86
1:A:189:MET:HE1	1:A:192:GLU:OE1	1.76	0.85
1:B:42:GLN:HG2	1:B:119:ILE:HD11	1.59	0.84
1:B:360:THR:HG22	1:B:362:GLY:H	1.43	0.84
1:A:250:ASN:HA	1:A:253:PHE:HB3	1.58	0.83
1:A:308:GLN:HE22	1:A:383:SER:H	1.24	0.83
1:C:106:ARG:HH12	1:C:367:SER:HA	1.45	0.82
1:C:276:LEU:HB2	1:C:281:TYR:HE1	1.42	0.82
1:B:265:ILE:HD11	1:B:448:MET:HG2	1.63	0.81
1:A:114:GLU:HB3	1:A:117:ARG:HH21	1.46	0.81
1:A:461:ARG:HG3	1:B:413:SER:OG	1.82	0.80
1:B:324:HIS:CD2	1:B:358:LEU:HD12	2.17	0.80
1:A:71:PHE:HE1	1:A:117:ARG:HA	1.48	0.79
1:B:96:ILE:HG13	1:B:109:ILE:HD12	1.62	0.79
1:B:231:GLN:NE2	1:B:269:SER:HB3	1.97	0.79
1:A:324:HIS:HD2	1:A:359:SER:H	1.30	0.79
1:C:231:GLN:NE2	1:C:269:SER:HB2	1.96	0.79
1:A:121:ARG:HH11	1:A:121:ARG:HG2	1.47	0.78
1:A:227:LYS:HE3	1:A:236:ARG:HB3	1.65	0.78
1:A:114:GLU:HA	1:A:117:ARG:HE	1.47	0.78
1:C:33:ILE:HD12	1:C:281:TYR:HE2	1.49	0.78
1:A:114:GLU:CB	1:A:117:ARG:HH21	1.97	0.77
1:A:272:HIS:CD2	1:B:411:THR:HA	2.19	0.77
1:A:340:ASP:O	1:A:343:VAL:HG12	1.85	0.77
1:C:154:LEU:HD21	1:C:167:MET:CE	2.15	0.77
1:A:483:ASN:N	1:A:483:ASN:HD22	1.82	0.77
1:A:317:ARG:HD3	1:A:369:GLU:OE1	1.84	0.76
1:B:317:ARG:HG2	1:B:320:GLU:OE2	1.85	0.76
1:A:390:THR:HG22	1:A:391:ARG:H	1.50	0.76
1:A:111:TYR:HB3	1:A:116:ILE:CD1	2.15	0.76
1:B:489:PHE:HB2	1:C:405:GLN:HG3	1.68	0.75
1:A:242:VAL:HG11	1:A:256:LEU:HD21	1.68	0.75
1:C:327:GLN:O	1:C:331:MET:HG3	1.84	0.75
1:B:217:ILE:HG13	1:B:218:ALA:N	2.02	0.75
1:B:21:ASN:HB3	1:B:24:GLU:HG3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ILE:HG13	1:B:218:ALA:H	1.49	0.75
1:C:422:ARG:HB3	1:C:423:PRO:HD3	1.68	0.75
1:C:276:LEU:HB2	1:C:281:TYR:CE1	2.21	0.74
1:A:174:ARG:N	1:A:174:ARG:HD3	2.03	0.74
1:C:353:VAL:CG2	1:C:354:PRO:HD2	2.17	0.74
1:A:232:THR:OG1	1:A:235:GLN:HG3	1.87	0.74
1:A:483:ASN:H	1:A:483:ASN:ND2	1.86	0.73
1:C:243:ARG:HG2	1:C:243:ARG:HH11	1.53	0.73
1:C:267:ARG:O	1:C:395:ASN:ND2	2.21	0.73
1:B:100:VAL:HG21	1:B:105:ARG:HD3	1.70	0.73
1:A:71:PHE:CE1	1:A:117:ARG:HA	2.24	0.73
1:C:299:VAL:O	1:C:388:ILE:HG23	1.89	0.73
1:B:160:ASP:HB3	1:B:163:MET:HG3	1.69	0.73
1:A:226:LEU:HD13	1:A:230:PHE:CE1	2.22	0.72
1:A:342:ARG:HB3	1:A:479:PHE:CE2	2.23	0.72
1:A:407:SER:OG	1:C:267:ARG:NH1	2.22	0.72
1:B:324:HIS:HD2	1:B:358:LEU:HD12	1.53	0.72
1:A:486:SER:HB3	1:B:408:ILE:HD11	1.70	0.72
1:C:270:VAL:HG12	1:C:271:ALA:N	2.05	0.72
1:A:163:MET:HE3	1:A:261:ARG:HG2	1.72	0.71
1:C:104:TRP:CZ2	1:C:376:SER:HB3	2.25	0.71
1:C:199:ARG:HH11	1:C:199:ARG:HG2	1.56	0.71
1:C:221:ARG:HG2	1:C:221:ARG:HH11	1.55	0.71
1:C:33:ILE:HG23	1:C:281:TYR:CD2	2.25	0.71
1:A:235:GLN:O	1:A:239:VAL:HG23	1.91	0.71
1:A:296:TYR:CD1	1:A:302:ASP:HB3	2.26	0.71
1:C:198:LYS:HD3	1:C:201:ILE:HD12	1.71	0.71
1:B:321:ASN:HD22	1:B:322:PRO:CD	2.03	0.71
1:A:324:HIS:CD2	1:A:359:SER:H	2.09	0.70
1:A:267:ARG:HG3	1:A:393:GLY:O	1.92	0.70
1:C:192:GLU:O	1:C:195:ARG:HG2	1.92	0.70
1:C:246:ARG:HH11	1:C:246:ARG:HG2	1.56	0.70
1:B:227:LYS:HB2	1:B:239:VAL:HG11	1.73	0.70
1:B:92:THR:HG22	1:B:93:GLY:N	2.07	0.70
1:B:21:ASN:HB2	1:B:24:GLU:HG3	1.73	0.69
1:A:489:PHE:HB2	1:B:405:GLN:HG3	1.74	0.69
1:B:155:VAL:HG23	1:B:156:ARG:N	2.06	0.69
1:C:289:TYR:CE1	1:C:294:GLU:HG2	2.27	0.69
1:C:63:ILE:O	1:C:67:VAL:HG23	1.92	0.69
1:A:453:PRO:HG3	1:B:420:PHE:CE1	2.28	0.69
1:B:321:ASN:HD22	1:B:322:PRO:HD2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLY:H	1:B:415:GLN:HE21	1.40	0.69
1:B:412:PHE:H	1:B:416:ARG:NH2	1.90	0.69
1:C:198:LYS:HA	1:C:201:ILE:HD12	1.74	0.69
1:A:37:GLY:HA3	1:A:285:VAL:HG21	1.75	0.69
1:A:340:ASP:HB2	1:B:408:ILE:HD13	1.74	0.69
1:B:138:ILE:HD12	1:B:183:VAL:HG21	1.76	0.69
1:C:93:GLY:HA3	1:C:110:LEU:HD23	1.75	0.68
1:C:154:LEU:HD21	1:C:167:MET:HE3	1.74	0.68
1:C:44:CYS:HA	1:C:49:LEU:HD12	1.75	0.68
1:A:92:THR:N	1:A:113:LYS:HG2	2.09	0.68
1:A:406:ILE:HD11	1:C:162:ARG:HD2	1.76	0.68
1:C:172:LEU:HD12	1:C:173:PRO:HD2	1.76	0.68
1:B:156:ARG:HH12	1:B:195:ARG:NH1	1.92	0.67
1:C:340:ASP:HB3	1:C:343:VAL:HG22	1.75	0.67
1:C:29:VAL:O	1:C:33:ILE:HG12	1.93	0.67
1:C:113:LYS:H	1:C:113:LYS:HD2	1.59	0.67
1:B:422:ARG:HB3	1:B:423:PRO:HD3	1.77	0.67
1:C:96:ILE:HG12	1:C:109:ILE:HG21	1.77	0.67
1:B:262:SER:HA	1:B:448:MET:CE	2.25	0.67
1:C:96:ILE:HG12	1:C:109:ILE:CG2	2.25	0.66
1:C:345:SER:HA	1:C:352:VAL:HG23	1.77	0.66
1:C:316:ILE:HD11	1:C:320:GLU:HB2	1.77	0.66
1:A:315:LEU:HD12	1:A:365:ILE:HD13	1.78	0.66
1:B:274:SER:OG	1:B:389:ARG:HD3	1.95	0.66
1:C:33:ILE:HG21	1:C:291:PHE:CD2	2.30	0.66
1:C:171:THR:HG22	1:C:171:THR:O	1.96	0.66
1:C:243:ARG:HG2	1:C:243:ARG:NH1	2.10	0.66
1:C:25:ILE:HG13	1:C:26:ARG:H	1.60	0.66
1:C:360:THR:HG22	1:C:362:GLY:H	1.60	0.66
1:A:375:GLU:OE1	1:A:375:GLU:N	2.30	0.65
1:C:98:ARG:O	1:C:105:ARG:N	2.27	0.65
1:A:151:THR:HG23	1:A:161:PRO:HB3	1.77	0.65
1:C:193:LEU:O	1:C:197:ILE:HG12	1.94	0.65
1:A:417:ASN:O	1:A:419:PRO:HD3	1.96	0.65
1:C:114:GLU:HG3	1:C:117:ARG:HH21	1.62	0.65
1:A:244:GLU:HA	1:A:244:GLU:OE1	1.95	0.65
1:C:109:ILE:CD1	1:C:111:TYR:HB2	2.27	0.65
1:A:26:ARG:HH11	1:A:295:GLY:HA3	1.62	0.65
1:C:325:LYS:HG2	1:C:360:THR:HG21	1.79	0.64
1:C:46:GLU:OE1	1:C:46:GLU:HA	1.97	0.64
1:B:162:ARG:HG2	1:C:404:GLY:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:OG	1:B:92:THR:HG21	1.97	0.64
1:A:242:VAL:HG13	1:A:252:GLU:HG3	1.78	0.64
1:C:410:PRO:HA	1:C:416:ARG:NH2	2.12	0.64
1:A:111:TYR:CB	1:A:116:ILE:HD11	2.26	0.64
1:B:95:PRO:HA	1:B:108:LEU:HD23	1.80	0.64
1:B:113:LYS:O	1:B:117:ARG:HB2	1.97	0.64
1:B:262:SER:HA	1:B:448:MET:HE1	1.80	0.64
1:A:227:LYS:HB2	1:A:239:VAL:HG11	1.79	0.63
1:C:422:ARG:HH11	1:C:422:ARG:HG2	1.64	0.63
1:A:62:THR:O	1:A:65:ARG:HG2	1.98	0.63
1:A:340:ASP:CB	1:B:408:ILE:HD13	2.29	0.63
1:C:194:ILE:HD12	1:C:253:PHE:HD1	1.64	0.63
1:A:342:ARG:HB3	1:A:479:PHE:CD2	2.34	0.62
1:C:340:ASP:OD1	1:C:486:SER:HB3	1.99	0.62
1:A:415:GLN:NE2	1:C:460:GLY:H	1.97	0.62
1:A:97:TYR:CE2	1:A:106:ARG:HG3	2.34	0.62
1:C:246:ARG:NH1	1:C:246:ARG:HG2	2.12	0.62
1:B:237:THR:HB	1:B:440:MET:SD	2.39	0.62
1:B:272:HIS:CD2	1:C:411:THR:HA	2.34	0.62
1:A:197:ILE:HG23	1:A:201:ILE:HG13	1.80	0.62
1:A:154:LEU:HD21	1:A:167:MET:HG2	1.81	0.62
1:C:221:ARG:HG2	1:C:221:ARG:NH1	2.14	0.62
1:A:344:SER:O	1:A:348:ARG:HB2	1.99	0.62
1:B:297:SER:O	1:B:303:PRO:HD3	1.99	0.62
1:A:180:GLY:O	1:A:183:VAL:HG12	2.00	0.61
1:A:176:SER:OG	1:A:180:GLY:HA3	1.99	0.61
1:B:120:TRP:CZ2	1:B:129:ALA:HB3	2.34	0.61
1:B:151:THR:O	1:B:155:VAL:HG13	2.00	0.61
1:C:151:THR:HA	1:C:154:LEU:HD12	1.81	0.61
1:A:121:ARG:HB3	1:A:126:GLY:HA2	1.82	0.61
1:C:265:ILE:HG13	1:C:266:LEU:H	1.65	0.61
1:B:238:MET:O	1:B:242:VAL:HG23	2.00	0.61
1:A:92:THR:N	1:A:113:LYS:HZ3	1.99	0.61
1:C:240:ASP:HA	1:C:243:ARG:NH1	2.14	0.61
1:A:58:GLN:HG3	1:A:315:LEU:CG	2.26	0.60
1:A:242:VAL:HG11	1:A:256:LEU:CD2	2.31	0.60
1:C:231:GLN:HG3	1:C:395:ASN:OD1	2.02	0.60
1:B:459:GLN:H	1:B:459:GLN:HE21	1.48	0.60
1:B:348:ARG:HH11	1:B:348:ARG:HG2	1.66	0.60
1:A:238:MET:HE1	1:A:259:LEU:HD13	1.83	0.60
1:B:346:PHE:CZ	1:B:477:PRO:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HD3	1:B:402:SER:HB2	1.83	0.60
1:A:255:ASP:O	1:A:258:PHE:HB3	2.02	0.60
1:C:154:LEU:HD21	1:C:167:MET:HE1	1.83	0.60
1:A:43:MET:O	1:A:47:LEU:HD23	2.02	0.59
1:B:464:PHE:CZ	1:B:471:ALA:HB1	2.37	0.59
1:C:380:GLU:OE2	1:C:382:ARG:HD3	2.02	0.59
1:C:265:ILE:HD11	1:C:448:MET:HE3	1.84	0.59
1:B:321:ASN:HB3	1:B:324:HIS:HB2	1.84	0.59
1:B:341:LEU:HD11	1:B:488:PHE:HA	1.84	0.59
1:B:265:ILE:HD11	1:B:448:MET:CG	2.31	0.59
1:A:339:GLU:HG3	1:B:411:THR:HB	1.83	0.59
1:C:270:VAL:O	1:C:391:ARG:HA	2.03	0.59
1:A:267:ARG:NH1	1:B:407:SER:OG	2.36	0.59
1:A:121:ARG:NH1	1:A:121:ARG:HG2	2.15	0.59
1:A:483:ASN:ND2	1:B:478:SER:HB2	2.17	0.59
1:C:199:ARG:HG2	1:C:199:ARG:NH1	2.18	0.59
1:B:411:THR:H	1:B:416:ARG:HH22	1.49	0.59
1:C:33:ILE:HG21	1:C:291:PHE:CE2	2.38	0.59
1:A:321:ASN:HB3	1:A:324:HIS:HB2	1.83	0.59
1:B:489:PHE:H	1:C:405:GLN:HE21	1.49	0.59
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.68	0.58
1:C:61:LEU:HA	1:C:64:GLU:OE1	2.03	0.58
1:C:283:SER:O	1:C:286:ALA:HB3	2.04	0.58
1:A:298:LEU:N	1:A:298:LEU:HD12	2.19	0.58
1:C:438:SER:HB3	1:C:441:ARG:HG3	1.84	0.58
1:C:216:ARG:NH2	1:C:243:ARG:O	2.37	0.58
1:A:150:ARG:O	1:A:154:LEU:HG	2.04	0.58
1:B:317:ARG:O	1:B:320:GLU:HB2	2.04	0.58
1:B:372:GLU:OE1	1:B:372:GLU:HA	2.04	0.58
1:B:115:GLU:OE1	1:B:115:GLU:HA	2.04	0.57
1:B:417:ASN:O	1:B:419:PRO:HD3	2.04	0.57
1:A:267:ARG:HB2	1:A:393:GLY:HA3	1.86	0.57
1:A:61:LEU:HA	1:A:64:GLU:OE1	2.04	0.57
1:C:324:HIS:CD2	1:C:359:SER:H	2.22	0.57
1:C:246:ARG:C	1:C:248:PRO:HD3	2.25	0.57
1:C:464:PHE:CD2	1:C:464:PHE:N	2.73	0.57
1:A:46:GLU:O	1:A:48:LYS:HG2	2.05	0.57
1:C:197:ILE:HD12	1:C:248:PRO:HB3	1.86	0.57
1:C:25:ILE:HG13	1:C:26:ARG:N	2.20	0.57
1:A:196:MET:CE	1:A:219:TYR:HB2	2.35	0.57
1:B:100:VAL:HG22	1:B:105:ARG:HD3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:HG2	1:B:489:PHE:HE2	1.68	0.57
1:B:139:TRP:CZ2	1:B:277:PRO:HG3	2.40	0.57
1:C:371:MET:HG2	1:C:371:MET:O	2.05	0.57
1:B:411:THR:N	1:B:416:ARG:HH22	2.03	0.56
1:A:238:MET:O	1:A:242:VAL:HG23	2.06	0.56
1:A:346:PHE:CE2	1:A:477:PRO:HB3	2.39	0.56
1:A:424:THR:O	1:A:427:ALA:HB3	2.05	0.56
1:A:390:THR:OG1	1:B:413:SER:HB2	2.05	0.56
1:C:240:ASP:O	1:C:244:GLU:HG2	2.03	0.56
1:A:71:PHE:CE1	1:A:117:ARG:HG2	2.40	0.56
1:B:155:VAL:HG23	1:B:156:ARG:H	1.69	0.56
1:C:109:ILE:HD11	1:C:111:TYR:HB2	1.88	0.56
1:B:366:ALA:HB3	1:B:369:GLU:HG3	1.87	0.56
1:A:321:ASN:HD22	1:A:322:PRO:HD2	1.70	0.56
1:B:321:ASN:OD1	1:B:324:HIS:ND1	2.37	0.56
1:B:346:PHE:CE2	1:B:477:PRO:HB3	2.41	0.56
1:C:190:VAL:HG13	1:C:256:LEU:HB3	1.88	0.56
1:A:339:GLU:OE1	1:A:340:ASP:N	2.35	0.56
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.71	0.56
1:C:475:ILE:O	1:C:477:PRO:HD3	2.05	0.56
1:A:189:MET:CE	1:A:192:GLU:OE1	2.52	0.55
1:A:31:LYS:HD3	1:A:292:GLU:OE2	2.05	0.55
1:A:321:ASN:HD22	1:A:322:PRO:CD	2.20	0.55
1:A:353:VAL:HG13	1:A:354:PRO:HD2	1.88	0.55
1:A:370:ASN:HD22	1:A:372:GLU:HB3	1.70	0.55
1:A:415:GLN:HE21	1:C:460:GLY:H	1.53	0.55
1:A:417:ASN:HA	1:C:455:ASP:O	2.06	0.55
1:A:230:PHE:HB3	1:A:235:GLN:HB3	1.88	0.55
1:B:134:THR:CG2	1:B:177:GLY:H	2.19	0.55
1:B:21:ASN:HB3	1:B:24:GLU:CG	2.35	0.55
1:B:39:PHE:CE2	1:B:67:VAL:HG21	2.42	0.55
1:A:263:ALA:HA	1:A:266:LEU:O	2.06	0.55
1:A:39:PHE:CZ	1:A:67:VAL:HG21	2.42	0.55
1:C:369:GLU:HG3	1:C:370:ASN:H	1.72	0.55
1:A:252:GLU:O	1:A:255:ASP:N	2.40	0.55
1:B:465:GLU:HB2	1:B:468:ASP:HB2	1.88	0.55
1:C:353:VAL:HG22	1:C:354:PRO:CD	2.32	0.55
1:A:311:GLN:HG3	1:A:313:TYR:CZ	2.42	0.55
1:B:231:GLN:HE22	1:B:269:SER:HB3	1.70	0.55
1:C:303:PRO:HG2	1:C:389:ARG:HH12	1.72	0.55
1:A:243:ARG:HG2	1:A:243:ARG:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ILE:HD11	1:C:256:LEU:HB2	1.89	0.54
1:A:253:PHE:CD2	1:A:253:PHE:C	2.81	0.54
1:A:97:TYR:N	1:A:97:TYR:CD1	2.74	0.54
1:B:190:VAL:O	1:B:194:ILE:HD13	2.08	0.54
1:C:198:LYS:HD3	1:C:201:ILE:CD1	2.37	0.54
1:C:270:VAL:CG1	1:C:271:ALA:N	2.69	0.54
1:B:56:LEU:HD11	1:B:315:LEU:HG	1.89	0.54
1:A:162:ARG:HD3	1:B:402:SER:CB	2.38	0.54
1:B:303:PRO:HG2	1:B:389:ARG:HH12	1.72	0.54
1:B:339:GLU:OE2	1:C:416:ARG:NH1	2.40	0.54
1:B:416:ARG:HD2	1:B:418:LEU:CD2	2.38	0.54
1:C:107:GLU:O	1:C:109:ILE:N	2.41	0.54
1:C:21:ASN:OD1	1:C:22:ALA:N	2.33	0.54
1:C:143:LEU:HA	1:C:332:ALA:CB	2.38	0.54
1:C:344:SER:O	1:C:347:ILE:HG22	2.08	0.53
1:C:38:ARG:HD2	1:C:123:ALA:O	2.08	0.53
1:C:348:ARG:NH2	1:C:380:GLU:O	2.40	0.53
1:C:46:GLU:C	1:C:48:LYS:H	2.11	0.53
1:C:58:GLN:HG3	1:C:315:LEU:HG	1.90	0.53
1:C:321:ASN:HB3	1:C:324:HIS:CD2	2.42	0.53
1:C:321:ASN:HB3	1:C:324:HIS:CG	2.43	0.53
1:C:348:ARG:HA	1:C:383:SER:OG	2.07	0.53
1:A:408:ILE:HD11	1:C:339:GLU:C	2.29	0.53
1:B:34:ASP:OD1	1:B:38:ARG:NH2	2.41	0.53
1:A:167:MET:HG3	1:A:170:SER:HB3	1.91	0.53
1:A:411:THR:O	1:C:389:ARG:HA	2.09	0.53
1:A:420:PHE:HA	1:C:487:TYR:OH	2.09	0.53
1:A:407:SER:HG	1:C:267:ARG:NH1	2.06	0.53
1:C:227:LYS:HB2	1:C:239:VAL:HG11	1.89	0.53
1:A:460:GLY:H	1:B:415:GLN:NE2	2.07	0.53
1:C:355:ARG:HB2	1:C:488:PHE:CE2	2.44	0.53
1:B:197:ILE:HG23	1:B:248:PRO:HB2	1.91	0.53
1:B:291:PHE:O	1:B:295:GLY:N	2.40	0.53
1:C:121:ARG:HB3	1:C:126:GLY:HA2	1.91	0.53
1:A:270:VAL:N	1:A:391:ARG:O	2.42	0.53
1:C:192:GLU:HB3	1:C:222:MET:HE1	1.89	0.53
1:C:267:ARG:HG3	1:C:393:GLY:O	2.09	0.53
1:C:33:ILE:HG23	1:C:281:TYR:CE2	2.43	0.53
1:B:355:ARG:HG2	1:B:489:PHE:CE2	2.43	0.52
1:A:196:MET:HE3	1:A:219:TYR:HB2	1.90	0.52
1:C:302:ASP:O	1:C:306:LEU:HD13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:O	1:A:236:ARG:HG3	2.09	0.52
1:A:339:GLU:OE1	1:B:416:ARG:NH1	2.43	0.52
1:A:134:THR:O	1:A:137:MET:HB3	2.10	0.52
1:A:100:VAL:HG12	1:A:101:ASP:N	2.22	0.52
1:A:71:PHE:CD1	1:A:117:ARG:HG2	2.44	0.52
1:A:370:ASN:ND2	1:A:372:GLU:HB3	2.24	0.52
1:C:174:ARG:HD3	1:C:175:ARG:H	1.75	0.52
1:C:270:VAL:HG12	1:C:271:ALA:H	1.74	0.52
1:B:265:ILE:HD11	1:B:448:MET:CB	2.39	0.52
1:C:342:ARG:HB3	1:C:479:PHE:CD2	2.45	0.52
1:A:100:VAL:O	1:A:101:ASP:C	2.48	0.52
1:A:69:SER:OG	1:A:92:THR:HG21	2.10	0.52
1:B:327:GLN:O	1:B:331:MET:HG3	2.09	0.52
1:B:69:SER:OG	1:B:92:THR:CG2	2.58	0.52
1:B:276:LEU:HD13	1:B:280:VAL:HG11	1.90	0.52
1:B:385:TYR:HB3	1:B:463:VAL:HG12	1.92	0.52
1:B:416:ARG:HD2	1:B:418:LEU:HD23	1.92	0.52
1:A:39:PHE:CE2	1:A:67:VAL:HG21	2.45	0.51
1:A:342:ARG:HH22	1:B:417:ASN:ND2	2.08	0.51
1:B:385:TYR:HB3	1:B:463:VAL:CG1	2.40	0.51
1:C:261:ARG:O	1:C:264:LEU:HB2	2.10	0.51
1:C:265:ILE:HD11	1:C:448:MET:CE	2.40	0.51
1:A:111:TYR:CD2	1:A:116:ILE:HD11	2.45	0.51
1:A:343:VAL:HG13	1:A:344:SER:N	2.24	0.51
1:A:315:LEU:HB2	1:A:365:ILE:HD11	1.92	0.51
1:C:61:LEU:HD23	1:C:64:GLU:OE1	2.09	0.51
1:A:317:ARG:HB2	1:A:320:GLU:HG3	1.91	0.51
1:A:35:GLY:HA3	1:A:124:ASN:OD1	2.11	0.51
1:B:155:VAL:CG2	1:B:156:ARG:N	2.71	0.51
1:B:406:ILE:O	1:B:420:PHE:HA	2.10	0.51
1:B:386:TRP:NE1	1:B:464:PHE:HB2	2.25	0.51
1:C:341:LEU:CB	1:C:486:SER:HA	2.32	0.51
1:A:296:TYR:CE1	1:A:302:ASP:HB3	2.46	0.51
1:C:231:GLN:HG3	1:C:395:ASN:CG	2.31	0.51
1:A:171:THR:O	1:A:173:PRO:HD3	2.11	0.51
1:B:343:VAL:HG23	1:B:344:SER:N	2.26	0.51
1:B:461:ARG:N	1:B:461:ARG:HD2	2.26	0.51
1:C:319:ASN:HD22	1:C:319:ASN:N	2.08	0.51
1:A:458:PHE:HB2	1:B:414:VAL:O	2.11	0.51
1:A:291:PHE:O	1:A:295:GLY:N	2.42	0.51
1:A:53:GLU:OE2	1:A:99:ARG:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ASN:HD22	1:B:322:PRO:N	2.09	0.51
1:C:422:ARG:HG2	1:C:422:ARG:NH1	2.26	0.51
1:B:408:ILE:O	1:B:408:ILE:HG22	2.09	0.51
1:C:57:ILE:HG22	1:C:58:GLN:N	2.26	0.51
1:A:38:ARG:NH1	1:A:123:ALA:O	2.44	0.50
1:A:253:PHE:O	1:A:257:ILE:HG13	2.11	0.50
1:C:421:ASP:OD1	1:C:424:THR:HG23	2.10	0.50
1:B:423:PRO:O	1:B:425:ILE:N	2.44	0.50
1:C:345:SER:CB	1:C:352:VAL:H	2.24	0.50
1:A:106:ARG:NH1	1:A:367:SER:HA	2.26	0.50
1:A:137:MET:CE	1:A:175:ARG:HE	2.25	0.50
1:A:168:GLN:O	1:A:184:LYS:HA	2.11	0.50
1:C:291:PHE:HE2	1:C:306:LEU:HD21	1.75	0.50
1:A:223:CYS:O	1:A:226:LEU:HB3	2.11	0.50
1:B:454:GLU:H	1:B:454:GLU:CD	2.15	0.50
1:A:29:VAL:O	1:A:32:MET:HG3	2.10	0.50
1:A:406:ILE:HG22	1:A:406:ILE:O	2.10	0.50
1:B:303:PRO:CG	1:B:389:ARG:HH12	2.24	0.50
1:B:324:HIS:HD2	1:B:358:LEU:HA	1.75	0.50
1:A:311:GLN:HG3	1:A:313:TYR:OH	2.12	0.50
1:C:250:ASN:HA	1:C:253:PHE:HB3	1.93	0.50
1:A:146:ALA:HB2	1:A:337:ALA:HB2	1.92	0.50
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.93	0.50
1:C:100:VAL:HG23	1:C:100:VAL:O	2.11	0.50
1:A:321:ASN:HD22	1:A:322:PRO:N	2.09	0.50
1:C:321:ASN:HD22	1:C:322:PRO:HD2	1.76	0.50
1:B:457:SER:O	1:C:415:GLN:HA	2.12	0.50
1:B:134:THR:HG23	1:B:177:GLY:H	1.76	0.50
1:B:60:SER:OG	1:B:278:ALA:HB3	2.11	0.50
1:A:308:GLN:HE22	1:A:383:SER:N	2.01	0.49
1:A:402:SER:HB3	1:C:162:ARG:NE	2.27	0.49
1:C:38:ARG:CD	1:C:123:ALA:O	2.60	0.49
1:C:394:GLY:O	1:C:395:ASN:O	2.30	0.49
1:C:37:GLY:O	1:C:41:ILE:HG13	2.12	0.49
1:A:483:ASN:ND2	1:B:476:VAL:O	2.46	0.49
1:C:100:VAL:O	1:C:103:LYS:O	2.30	0.49
1:A:118:ARG:HH21	1:A:122:GLN:HG3	1.77	0.49
1:B:316:ILE:CG1	1:B:320:GLU:HB3	2.42	0.49
1:C:300:GLY:O	1:C:303:PRO:HD2	2.12	0.49
1:C:410:PRO:HA	1:C:416:ARG:HH21	1.77	0.49
1:B:452:ARG:NH1	1:C:449:GLU:OE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HE21	1:A:58:GLN:HA	1.77	0.49
1:B:30:GLY:O	1:B:34:ASP:HB2	2.12	0.49
1:C:243:ARG:O	1:C:243:ARG:HG3	2.11	0.49
1:A:483:ASN:HD21	1:B:478:SER:HB2	1.77	0.49
1:B:488:PHE:H	1:C:405:GLN:NE2	2.11	0.49
1:C:196:MET:O	1:C:197:ILE:C	2.50	0.49
1:C:104:TRP:CZ2	1:C:376:SER:CB	2.96	0.49
1:B:339:GLU:C	1:C:408:ILE:HD11	2.33	0.49
1:A:162:ARG:HG2	1:B:404:GLY:O	2.13	0.49
1:C:195:ARG:CG	1:C:196:MET:N	2.76	0.49
1:C:289:TYR:CZ	1:C:294:GLU:HG2	2.48	0.49
1:C:291:PHE:CE2	1:C:306:LEU:HD21	2.48	0.49
1:C:143:LEU:HA	1:C:332:ALA:HB1	1.95	0.49
1:C:33:ILE:HD12	1:C:281:TYR:CE2	2.40	0.49
1:A:406:ILE:HG23	1:A:421:ASP:HB3	1.94	0.49
1:C:52:TYR:HE2	1:C:104:TRP:HH2	1.59	0.49
1:B:234:ALA:HB1	1:B:444:ILE:CG1	2.41	0.48
1:B:92:THR:CG2	1:B:93:GLY:N	2.74	0.48
1:C:22:ALA:O	1:C:25:ILE:HG12	2.13	0.48
1:B:37:GLY:O	1:B:41:ILE:HG13	2.13	0.48
1:A:166:LEU:HD21	1:A:264:LEU:HD23	1.95	0.48
1:B:190:VAL:HG13	1:B:256:LEU:HB3	1.94	0.48
1:B:326:SER:HA	1:B:379:LEU:HD22	1.96	0.48
1:A:267:ARG:HH21	1:B:418:LEU:HB2	1.77	0.48
1:C:43:MET:CE	1:C:119:ILE:HG21	2.44	0.48
1:C:171:THR:CG2	1:C:171:THR:O	2.60	0.48
1:C:370:ASN:OD1	1:C:373:THR:HG23	2.12	0.48
1:A:298:LEU:CD1	1:A:298:LEU:N	2.76	0.48
1:A:345:SER:HA	1:A:352:VAL:HG23	1.96	0.48
1:A:63:ILE:O	1:A:67:VAL:HG23	2.12	0.48
1:C:252:GLU:H	1:C:252:GLU:CD	2.17	0.48
1:A:56:LEU:HG	1:A:58:GLN:HG2	1.95	0.48
1:B:168:GLN:O	1:B:184:LYS:HA	2.13	0.48
1:B:321:ASN:ND2	1:B:322:PRO:HD2	2.27	0.48
1:B:43:MET:CE	1:B:43:MET:HA	2.44	0.48
1:B:453:PRO:O	1:C:417:ASN:HB2	2.12	0.48
1:B:97:TYR:N	1:B:97:TYR:CD1	2.81	0.48
1:C:98:ARG:NE	1:C:107:GLU:OE2	2.44	0.48
1:C:113:LYS:H	1:C:113:LYS:CD	2.22	0.48
1:C:265:ILE:HG13	1:C:266:LEU:N	2.27	0.48
1:A:189:MET:HB2	1:A:226:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:HG22	1:B:194:ILE:HG21	1.96	0.48
1:C:321:ASN:HD22	1:C:322:PRO:CD	2.26	0.48
1:B:156:ARG:NH1	1:B:195:ARG:NH1	2.61	0.48
1:B:258:PHE:O	1:B:261:ARG:HB3	2.14	0.48
1:C:174:ARG:HD3	1:C:175:ARG:N	2.28	0.48
1:C:477:PRO:HB2	1:C:479:PHE:CE1	2.49	0.48
1:C:340:ASP:HA	1:C:486:SER:HB2	1.96	0.48
1:B:214:ARG:HG2	1:B:214:ARG:NH1	2.27	0.47
1:B:455:ASP:O	1:C:417:ASN:HA	2.13	0.47
1:C:121:ARG:O	1:C:126:GLY:N	2.37	0.47
1:C:341:LEU:HD12	1:C:485:GLY:O	2.14	0.47
1:B:37:GLY:HA2	1:B:282:GLY:N	2.29	0.47
1:B:386:TRP:HB3	1:B:466:LEU:CD2	2.43	0.47
1:A:477:PRO:HG3	1:B:414:VAL:HG11	1.96	0.47
1:C:297:SER:O	1:C:303:PRO:HG3	2.14	0.47
1:B:143:LEU:HD11	1:B:363:VAL:HG21	1.97	0.47
1:C:22:ALA:O	1:C:25:ILE:CG1	2.62	0.47
1:C:230:PHE:CD1	1:C:235:GLN:HB3	2.49	0.47
1:A:226:LEU:HD12	1:A:239:VAL:HG13	1.96	0.47
1:A:318:PRO:HD3	1:A:373:THR:O	2.14	0.47
1:B:293:ARG:HG3	1:B:293:ARG:HH11	1.80	0.47
1:B:124:ASN:O	1:B:127:ASP:OD2	2.32	0.47
1:C:406:ILE:HG13	1:C:421:ASP:HB3	1.95	0.47
1:B:92:THR:OG1	1:B:113:LYS:HG2	2.15	0.47
1:B:348:ARG:HG2	1:B:348:ARG:NH1	2.29	0.47
1:B:62:THR:HG23	1:B:94:GLY:HA3	1.97	0.47
1:C:247:ASN:O	1:C:248:PRO:C	2.53	0.47
1:A:316:ILE:HG22	1:A:376:SER:HA	1.95	0.47
1:B:166:LEU:HB3	1:B:187:GLY:H	1.78	0.47
1:B:449:GLU:OE2	1:C:446:ARG:NH1	2.40	0.47
1:C:208:ARG:HH11	1:C:208:ARG:HG2	1.80	0.47
1:A:40:TYR:CE2	1:A:279:CYS:HA	2.50	0.47
1:A:297:SER:C	1:A:298:LEU:HD12	2.35	0.47
1:A:443:GLU:O	1:A:447:LEU:HG	2.15	0.47
1:B:155:VAL:CG2	1:B:156:ARG:H	2.27	0.47
1:C:115:GLU:OE2	1:C:118:ARG:NH2	2.48	0.47
1:C:141:SER:OG	1:C:169:GLY:HA2	2.14	0.47
1:C:143:LEU:HD12	1:C:143:LEU:O	2.13	0.47
1:C:49:LEU:HD22	1:C:53:GLU:HB3	1.97	0.47
1:A:174:ARG:HD3	1:A:175:ARG:H	1.80	0.47
1:C:258:PHE:HE2	1:C:444:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:HH12	1:A:367:SER:HA	1.79	0.47
1:A:368:ASN:N	1:A:368:ASN:HD22	2.13	0.47
1:B:190:VAL:HG12	1:B:194:ILE:HD13	1.97	0.47
1:C:135:HIS:HE1	1:C:298:LEU:CD2	2.27	0.47
1:C:106:ARG:NH1	1:C:367:SER:HA	2.22	0.47
1:C:92:THR:HG21	1:C:116:ILE:HD12	1.96	0.47
1:B:343:VAL:HG11	1:C:416:ARG:HH11	1.80	0.47
1:C:345:SER:HB3	1:C:352:VAL:H	1.79	0.47
1:A:267:ARG:HH21	1:B:418:LEU:CB	2.27	0.46
1:C:385:TYR:HB3	1:C:463:VAL:CG1	2.45	0.46
1:A:143:LEU:HA	1:A:332:ALA:HB2	1.96	0.46
1:A:297:SER:O	1:A:303:PRO:HG3	2.16	0.46
1:A:386:TRP:NE1	1:A:464:PHE:HB2	2.30	0.46
1:B:96:ILE:HG13	1:B:109:ILE:CD1	2.40	0.46
1:C:438:SER:HB3	1:C:441:ARG:CG	2.44	0.46
1:A:170:SER:HA	1:A:188:THR:HG23	1.97	0.46
1:A:304:PHE:CE2	1:A:386:TRP:HA	2.50	0.46
1:B:93:GLY:HA2	1:B:109:ILE:O	2.15	0.46
1:C:265:ILE:CG1	1:C:266:LEU:H	2.29	0.46
1:A:342:ARG:HB3	1:A:479:PHE:HE2	1.73	0.46
1:B:302:ASP:N	1:B:303:PRO:HD2	2.31	0.46
1:C:204:ARG:O	1:C:205:ASN:HB2	2.15	0.46
1:A:39:PHE:CZ	1:A:67:VAL:CG2	2.99	0.46
1:A:487:TYR:HB3	1:B:405:GLN:HB2	1.96	0.46
1:C:129:ALA:O	1:C:133:LEU:HG	2.16	0.46
1:C:164:CYS:C	1:C:166:LEU:N	2.68	0.46
1:B:300:GLY:O	1:B:303:PRO:HD2	2.16	0.46
1:B:296:TYR:CE1	1:B:302:ASP:HB3	2.51	0.46
1:C:111:TYR:HB3	1:C:116:ILE:HD11	1.97	0.46
1:C:24:GLU:O	1:C:25:ILE:C	2.54	0.46
1:B:393:GLY:HA2	1:C:410:PRO:HG3	1.97	0.46
1:C:457:SER:O	1:C:458:PHE:HB2	2.16	0.46
1:A:163:MET:CE	1:A:261:ARG:HG2	2.43	0.46
1:B:58:GLN:HG3	1:B:315:LEU:HD12	1.98	0.46
1:A:232:THR:OG1	1:A:235:GLN:CG	2.61	0.46
1:A:324:HIS:HD2	1:A:358:LEU:HA	1.81	0.46
1:A:56:LEU:O	1:A:57:ILE:C	2.54	0.46
1:B:193:LEU:HA	1:B:222:MET:HE3	1.98	0.46
1:B:234:ALA:HB1	1:B:444:ILE:HG12	1.97	0.46
1:C:56:LEU:HD22	1:C:104:TRP:CZ3	2.50	0.46
1:A:53:GLU:OE2	1:A:98:ARG:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ASP:OD2	1:C:291:PHE:HB2	2.16	0.45
1:C:95:PRO:HB2	1:C:97:TYR:HE2	1.81	0.45
1:A:402:SER:HB3	1:C:162:ARG:CZ	2.47	0.45
1:C:164:CYS:O	1:C:166:LEU:N	2.49	0.45
1:A:143:LEU:HA	1:A:332:ALA:CB	2.47	0.45
1:C:406:ILE:HD11	1:C:425:ILE:HG13	1.99	0.45
1:B:232:THR:OG1	1:B:235:GLN:HG3	2.16	0.45
1:B:301:ILE:O	1:B:302:ASP:C	2.54	0.45
1:B:276:LEU:HD22	1:B:307:LEU:HD21	1.99	0.45
1:C:205:ASN:ND2	1:C:205:ASN:N	2.64	0.45
1:C:247:ASN:N	1:C:248:PRO:HD3	2.31	0.45
1:C:270:VAL:CG1	1:C:271:ALA:H	2.29	0.45
1:B:170:SER:HA	1:B:188:THR:HG23	1.99	0.45
1:C:33:ILE:HG23	1:C:281:TYR:HD2	1.79	0.45
1:A:269:SER:HA	1:A:391:ARG:O	2.17	0.45
1:C:215:THR:O	1:C:218:ALA:N	2.50	0.45
1:B:193:LEU:O	1:B:197:ILE:HG12	2.16	0.45
1:B:255:ASP:O	1:B:258:PHE:HB3	2.17	0.45
1:A:232:THR:HG1	1:A:235:GLN:HG3	1.80	0.45
1:A:56:LEU:O	1:A:58:GLN:N	2.49	0.45
1:B:141:SER:HB2	1:B:172:LEU:HD12	1.98	0.45
1:C:230:PHE:CE1	1:C:259:LEU:HD12	2.52	0.45
1:C:356:GLY:O	1:C:357:LYS:HG3	2.17	0.45
1:A:92:THR:CA	1:A:113:LYS:HZ3	2.30	0.45
1:A:174:ARG:CD	1:A:175:ARG:H	2.30	0.45
1:B:232:THR:CG2	1:B:235:GLN:HE21	2.30	0.45
1:B:451:ALA:O	1:B:452:ARG:HD3	2.17	0.45
1:C:25:ILE:O	1:C:29:VAL:HG23	2.17	0.45
1:A:39:PHE:CE1	1:A:43:MET:HE2	2.52	0.44
1:C:456:VAL:HG13	1:C:456:VAL:O	2.17	0.44
1:C:58:GLN:HE21	1:C:58:GLN:HA	1.82	0.44
1:A:111:TYR:HD2	1:A:116:ILE:HD11	1.81	0.44
1:C:116:ILE:O	1:C:119:ILE:HG22	2.16	0.44
1:C:193:LEU:HD21	1:C:222:MET:HB2	1.98	0.44
1:A:487:TYR:CD2	1:A:487:TYR:N	2.84	0.44
1:A:68:LEU:HD21	1:A:133:LEU:O	2.17	0.44
1:C:30:GLY:HA2	1:C:291:PHE:HB3	1.98	0.44
1:C:135:HIS:CE1	1:C:298:LEU:HD21	2.53	0.44
1:C:44:CYS:SG	1:C:49:LEU:HD12	2.58	0.44
1:C:58:GLN:CA	1:C:58:GLN:HE21	2.29	0.44
1:A:483:ASN:N	1:A:483:ASN:ND2	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLY:CA	1:B:282:GLY:HA2	2.47	0.44
1:B:408:ILE:HD12	1:B:419:PRO:HB2	1.98	0.44
1:A:34:ASP:OD2	1:A:291:PHE:HB2	2.17	0.44
1:C:301:ILE:HG12	1:C:305:ARG:HG3	1.99	0.44
1:C:58:GLN:HE22	1:C:363:VAL:HG13	1.81	0.44
1:A:386:TRP:CE2	1:A:464:PHE:HB2	2.53	0.44
1:B:41:ILE:HD11	1:B:286:ALA:N	2.32	0.44
1:C:160:ASP:O	1:C:163:MET:HG3	2.18	0.44
1:C:247:ASN:HD22	1:C:247:ASN:C	2.20	0.44
1:A:47:LEU:HD11	1:A:109:ILE:CD1	2.48	0.44
1:A:342:ARG:HH22	1:B:417:ASN:HD21	1.65	0.44
1:C:406:ILE:O	1:C:406:ILE:HG12	2.18	0.44
1:C:422:ARG:HB3	1:C:423:PRO:CD	2.45	0.44
1:C:438:SER:HB3	1:C:441:ARG:CD	2.47	0.44
1:C:262:SER:HA	1:C:448:MET:CE	2.47	0.44
1:A:197:ILE:HG23	1:A:201:ILE:CG1	2.45	0.44
1:A:50:SER:OG	1:A:53:GLU:HG3	2.18	0.44
1:B:269:SER:HB2	1:B:391:ARG:O	2.17	0.44
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.83	0.44
1:C:485:GLY:O	1:C:487:TYR:N	2.51	0.44
1:A:172:LEU:HD12	1:A:173:PRO:HD2	2.00	0.44
1:A:26:ARG:NH1	1:A:295:GLY:C	2.71	0.44
1:B:118:ARG:HD2	1:B:119:ILE:N	2.33	0.44
1:A:416:ARG:HG2	1:C:343:VAL:HG11	1.99	0.44
1:A:114:GLU:HA	1:A:117:ARG:NE	2.24	0.43
1:A:185:GLY:HA2	1:A:270:VAL:HG21	2.00	0.43
1:B:459:GLN:H	1:B:459:GLN:NE2	2.14	0.43
1:C:204:ARG:O	1:C:205:ASN:CB	2.66	0.43
1:B:343:VAL:HG11	1:C:416:ARG:CD	2.47	0.43
1:B:63:ILE:O	1:B:67:VAL:HG23	2.18	0.43
1:C:98:ARG:HB2	1:C:105:ARG:HB2	1.99	0.43
1:A:145:ASP:OD2	1:A:169:GLY:N	2.48	0.43
1:B:312:VAL:O	1:B:379:LEU:HB2	2.18	0.43
1:C:58:GLN:CA	1:C:58:GLN:NE2	2.81	0.43
1:C:61:LEU:HD12	1:C:364:GLN:HG2	2.00	0.43
1:B:100:VAL:O	1:B:101:ASP:C	2.56	0.43
1:B:384:ARG:HH11	1:B:384:ARG:HG2	1.84	0.43
1:C:195:ARG:HG2	1:C:196:MET:N	2.33	0.43
1:C:240:ASP:HA	1:C:243:ARG:HH12	1.80	0.43
1:C:61:LEU:O	1:C:65:ARG:HG3	2.18	0.43
1:B:235:GLN:O	1:B:239:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:O	1:C:48:LYS:N	2.51	0.43
1:A:51:ASP:O	1:A:55:ARG:HG3	2.19	0.43
1:B:115:GLU:CA	1:B:115:GLU:OE1	2.66	0.43
1:A:420:PHE:CD1	1:C:265:ILE:HG22	2.53	0.43
1:C:320:GLU:OE1	1:C:325:LYS:NZ	2.51	0.43
1:C:446:ARG:O	1:C:449:GLU:HB3	2.19	0.43
1:B:37:GLY:HA2	1:B:282:GLY:CA	2.49	0.43
1:B:39:PHE:CZ	1:B:67:VAL:CG2	3.01	0.43
1:C:164:CYS:C	1:C:166:LEU:H	2.21	0.43
1:B:103:LYS:HD3	1:B:372:GLU:OE1	2.18	0.43
1:C:216:ARG:NH1	1:C:245:SER:O	2.49	0.43
1:C:32:MET:O	1:C:36:ILE:HG13	2.19	0.43
1:C:462:GLY:O	1:C:464:PHE:CE2	2.71	0.43
1:B:327:GLN:NE2	1:B:353:VAL:O	2.49	0.43
1:B:238:MET:HE2	1:B:440:MET:HB2	2.01	0.43
1:C:194:ILE:HD12	1:C:253:PHE:CD1	2.49	0.43
1:C:338:PHE:CD1	1:C:338:PHE:N	2.87	0.43
1:C:382:ARG:NH1	1:C:382:ARG:HG2	2.33	0.43
1:C:52:TYR:HE2	1:C:104:TRP:CH2	2.36	0.43
1:A:235:GLN:HE21	1:A:266:LEU:HB2	1.83	0.42
1:A:33:ILE:HG22	1:A:34:ASP:N	2.34	0.42
1:A:223:CYS:O	1:A:227:LYS:N	2.45	0.42
1:B:193:LEU:HD23	1:B:222:MET:HE2	2.01	0.42
1:B:242:VAL:HG12	1:B:242:VAL:O	2.20	0.42
1:C:97:TYR:HA	1:C:105:ARG:O	2.19	0.42
1:A:303:PRO:HD2	1:A:389:ARG:HH22	1.84	0.42
1:A:37:GLY:HA3	1:A:285:VAL:CG2	2.46	0.42
1:A:40:TYR:CE1	1:A:63:ILE:HD12	2.54	0.42
1:A:453:PRO:HG3	1:B:420:PHE:CD1	2.53	0.42
1:C:438:SER:HB3	1:C:441:ARG:HD2	2.01	0.42
1:A:58:GLN:CA	1:A:58:GLN:HE21	2.31	0.42
1:C:120:TRP:CZ2	1:C:129:ALA:HB3	2.55	0.42
1:C:139:TRP:CZ2	1:C:143:LEU:HD22	2.54	0.42
1:A:33:ILE:HG21	1:A:291:PHE:CG	2.54	0.42
1:C:317:ARG:HB2	1:C:318:PRO:HD2	2.01	0.42
1:B:343:VAL:HG11	1:C:416:ARG:HD3	2.01	0.42
1:A:417:ASN:C	1:A:417:ASN:OD1	2.58	0.42
1:A:58:GLN:NE2	1:A:58:GLN:HA	2.34	0.42
1:C:213:ARG:O	1:C:217:ILE:HG13	2.19	0.42
1:C:237:THR:O	1:C:241:GLN:HG3	2.19	0.42
1:C:316:ILE:HG13	1:C:320:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MET:SD	1:A:191:MET:HG3	2.60	0.42
1:A:452:ARG:HA	1:A:453:PRO:HD3	1.95	0.42
1:C:265:ILE:CG1	1:C:266:LEU:N	2.83	0.42
1:A:112:ASP:O	1:A:113:LYS:C	2.56	0.42
1:A:124:ASN:O	1:A:127:ASP:HB2	2.20	0.42
1:A:221:ARG:O	1:A:224:ASN:N	2.53	0.42
1:A:317:ARG:HB2	1:A:320:GLU:CG	2.49	0.42
1:B:114:GLU:HA	1:B:117:ARG:NE	2.34	0.42
1:B:238:MET:SD	1:B:259:LEU:CD1	3.08	0.42
1:B:92:THR:HG22	1:B:93:GLY:H	1.80	0.42
1:C:172:LEU:HD12	1:C:172:LEU:HA	1.88	0.42
1:C:361:ARG:HD3	1:C:361:ARG:HA	1.80	0.42
1:A:174:ARG:HD3	1:A:174:ARG:H	1.82	0.42
1:A:230:PHE:CE2	1:A:259:LEU:HG	2.55	0.42
1:A:317:ARG:HB3	1:A:318:PRO:HD2	2.01	0.42
1:B:320:GLU:OE1	1:B:360:THR:HG23	2.19	0.42
1:C:342:ARG:C	1:C:344:SER:H	2.23	0.42
1:C:370:ASN:ND2	1:C:372:GLU:H	2.18	0.42
1:C:60:SER:HB3	1:C:279:CYS:HB3	2.02	0.42
1:A:114:GLU:HB3	1:A:117:ARG:NH2	2.26	0.42
1:A:122:GLN:OE1	1:A:122:GLN:HA	2.20	0.42
1:A:424:THR:O	1:A:427:ALA:CB	2.68	0.42
1:A:60:SER:O	1:A:64:GLU:HG3	2.20	0.42
1:B:149:GLN:HG2	1:B:151:THR:HG23	2.02	0.42
1:B:68:LEU:C	1:B:175:ARG:HH22	2.22	0.42
1:B:68:LEU:HB3	1:B:175:ARG:NH2	2.34	0.42
1:C:192:GLU:HA	1:C:195:ARG:HD3	2.00	0.42
1:C:265:ILE:HD11	1:C:448:MET:CG	2.50	0.42
1:B:343:VAL:HG21	1:C:416:ARG:NH1	2.34	0.42
1:A:230:PHE:CZ	1:A:259:LEU:HG	2.55	0.41
1:A:346:PHE:HE2	1:A:463:VAL:HG21	1.85	0.41
1:A:324:HIS:CD2	1:A:358:LEU:HA	2.55	0.41
1:B:317:ARG:H	1:B:317:ARG:HG2	1.62	0.41
1:B:395:ASN:HD22	1:B:395:ASN:C	2.22	0.41
1:B:234:ALA:CB	1:B:444:ILE:HG12	2.50	0.41
1:C:150:ARG:HD3	1:C:150:ARG:HA	1.81	0.41
1:C:46:GLU:C	1:C:48:LYS:N	2.72	0.41
1:B:217:ILE:CG1	1:B:218:ALA:H	2.28	0.41
1:B:273:LYS:HB3	1:B:298:LEU:HD23	2.01	0.41
1:B:64:GLU:O	1:B:68:LEU:HG	2.20	0.41
1:C:134:THR:HA	1:C:137:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:HD2	1:A:253:PHE:C	2.21	0.41
1:B:303:PRO:HG2	1:B:389:ARG:NH1	2.35	0.41
1:B:423:PRO:O	1:B:424:THR:C	2.57	0.41
1:C:341:LEU:HD23	1:C:341:LEU:HA	1.91	0.41
1:C:464:PHE:CE1	1:C:471:ALA:HB1	2.55	0.41
1:C:265:ILE:HD11	1:C:448:MET:HG2	2.03	0.41
1:C:385:TYR:HB3	1:C:463:VAL:HG12	2.02	0.41
1:C:56:LEU:HG	1:C:58:GLN:HG2	2.02	0.41
1:B:386:TRP:HB3	1:B:466:LEU:HD21	2.02	0.41
1:C:166:LEU:HB3	1:C:187:GLY:H	1.86	0.41
1:A:151:THR:O	1:A:155:VAL:HG22	2.20	0.41
1:C:113:LYS:HD2	1:C:113:LYS:N	2.30	0.41
1:C:342:ARG:C	1:C:344:SER:N	2.73	0.41
1:A:264:LEU:O	1:A:267:ARG:NH1	2.54	0.41
1:A:473:SER:HA	1:A:474:PRO:HD3	1.63	0.41
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.36	0.41
1:C:174:ARG:HD3	1:C:174:ARG:N	2.36	0.41
1:C:324:HIS:HD2	1:C:359:SER:H	1.67	0.41
1:C:265:ILE:HD11	1:C:448:MET:HB3	2.03	0.41
1:B:217:ILE:CG1	1:B:218:ALA:N	2.79	0.41
1:B:41:ILE:CD1	1:B:286:ALA:HB2	2.51	0.41
1:A:272:HIS:NE2	1:B:410:PRO:O	2.51	0.41
1:B:62:THR:O	1:B:66:MET:HG3	2.21	0.41
1:C:255:ASP:O	1:C:258:PHE:HB3	2.21	0.41
1:A:155:VAL:HG12	1:A:161:PRO:HD3	2.03	0.40
1:A:238:MET:CE	1:A:255:ASP:OD1	2.69	0.40
1:A:257:ILE:O	1:A:260:ALA:HB3	2.21	0.40
1:A:315:LEU:HD12	1:A:365:ILE:CD1	2.50	0.40
1:B:66:MET:HA	1:B:92:THR:HG21	2.02	0.40
1:A:157:THR:HB	1:A:159:MET:HG3	2.04	0.40
1:A:321:ASN:HD22	1:A:321:ASN:C	2.24	0.40
1:A:406:ILE:HG23	1:A:421:ASP:CB	2.51	0.40
1:A:407:SER:OG	1:A:408:ILE:N	2.54	0.40
1:B:238:MET:SD	1:B:259:LEU:HD11	2.62	0.40
1:C:34:ASP:O	1:C:38:ARG:HG3	2.22	0.40
1:C:104:TRP:HZ2	1:C:376:SER:CB	2.35	0.40
1:C:97:TYR:CD2	1:C:97:TYR:N	2.88	0.40
1:A:121:ARG:O	1:A:122:GLN:C	2.60	0.40
1:A:239:VAL:HG22	1:A:259:LEU:HD21	2.04	0.40
1:A:302:ASP:N	1:A:303:PRO:CD	2.84	0.40
1:A:408:ILE:HD11	1:C:340:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLN:NE2	1:B:269:SER:CB	2.78	0.40
1:B:339:GLU:OE2	1:B:343:VAL:HG21	2.21	0.40
1:A:238:MET:HE3	1:A:255:ASP:OD1	2.21	0.40
1:B:160:ASP:C	1:B:162:ARG:H	2.24	0.40
1:B:358:LEU:HD12	1:B:358:LEU:HA	1.97	0.40
1:C:121:ARG:HG3	1:C:121:ARG:HH11	1.86	0.40
1:C:205:ASN:N	1:C:205:ASN:HD22	2.17	0.40
1:C:21:ASN:CG	1:C:22:ALA:H	2.09	0.40
1:C:235:GLN:O	1:C:239:VAL:HG23	2.20	0.40
1:C:331:MET:SD	1:C:488:PHE:CE1	3.15	0.40
1:A:168:GLN:NE2	1:A:183:VAL:HG22	2.36	0.40
1:C:195:ARG:HG2	1:C:196:MET:H	1.87	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	416/499 (83%)	361 (87%)	50 (12%)	5 (1%)	15	56
1	B	416/499 (83%)	360 (86%)	43 (10%)	13 (3%)	5	31
1	C	428/499 (86%)	349 (82%)	68 (16%)	11 (3%)	6	36
All	All	1260/1497 (84%)	1070 (85%)	161 (13%)	29 (2%)	7	40

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	423	PRO
1	C	203	ASP
1	C	395	ASN
1	C	486	SER
1	A	233	ALA

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Mol	Chain	Res	Type
1	A	472	THR
1	B	150	ARG
1	B	177	GLY
1	B	424	THR
1	C	25	ILE
1	A	101	ASP
1	A	250	ASN
1	B	101	ASP
1	B	341	LEU
1	C	108	LEU
1	C	421	ASP
1	C	480	ASP
1	B	340	ASP
1	B	469	GLU
1	A	448	MET
1	B	318	PRO
1	C	47	LEU
1	C	266	LEU
1	B	427	ALA
1	C	406	ILE
1	C	423	PRO
1	B	248	PRO
1	B	425	ILE
1	B	356	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/425 (85%)	336 (93%)	26 (7%)	17	53
1	B	362/425 (85%)	342 (94%)	20 (6%)	25	64
1	C	370/425 (87%)	343 (93%)	27 (7%)	16	53
All	All	1094/1275 (86%)	1021 (93%)	73 (7%)	19	56

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	32	MET
1	A	33	ILE
1	A	48	LYS
1	A	106	ARG
1	A	108	LEU
1	A	111	TYR
1	A	112	ASP
1	A	118	ARG
1	A	139	TRP
1	A	174	ARG
1	A	191	MET
1	A	202	ASN
1	A	244	GLU
1	A	246	ARG
1	A	253	PHE
1	A	267	ARG
1	A	321	ASN
1	A	339	GLU
1	A	348	ARG
1	A	384	ARG
1	A	390	THR
1	A	416	ARG
1	A	456	VAL
1	A	483	ASN
1	A	484	GLU
1	B	21	ASN
1	B	58	GLN
1	B	107	GLU
1	B	114	GLU
1	B	139	TRP
1	B	174	ARG
1	B	220	GLU
1	B	305	ARG
1	B	308	GLN
1	B	317	ARG
1	B	321	ASN
1	B	368	ASN
1	B	389	ARG
1	B	390	THR
1	B	395	ASN
1	B	438	SER
1	B	459	GLN

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Mol	Chain	Res	Type
1	B	461	ARG
1	B	479	PHE
1	B	483	ASN
1	C	46	GLU
1	C	57	ILE
1	C	58	GLN
1	C	59	ASN
1	C	60	SER
1	C	99	ARG
1	C	105	ARG
1	C	109	ILE
1	C	113	LYS
1	C	174	ARG
1	C	226	LEU
1	C	243	ARG
1	C	247	ASN
1	C	255	ASP
1	C	314	SER
1	C	321	ASN
1	C	371	MET
1	C	372	GLU
1	C	375	GLU
1	C	382	ARG
1	C	389	ARG
1	C	390	THR
1	C	441	ARG
1	C	446	ARG
1	C	469	GLU
1	C	481	MET
1	C	483	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	224	ASN
1	A	308	GLN
1	A	319	ASN
1	A	321	ASN
1	A	324	HIS
1	A	368	ASN
1	A	370	ASN

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Mol	Chain	Res	Type
1	A	405	GLN
1	A	415	GLN
1	A	483	ASN
1	B	122	GLN
1	B	142	ASN
1	B	231	GLN
1	B	235	GLN
1	B	241	GLN
1	B	308	GLN
1	B	309	ASN
1	B	311	GLN
1	B	321	ASN
1	B	395	ASN
1	B	415	GLN
1	B	459	GLN
1	B	483	ASN
1	C	140	HIS
1	C	142	ASN
1	C	205	ASN
1	C	247	ASN
1	C	308	GLN
1	C	309	ASN
1	C	319	ASN
1	C	321	ASN
1	C	324	HIS
1	C	370	ASN
1	C	405	GLN
1	C	459	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	425/499 (85%)	-0.03	4 (0%) 84 75	31, 69, 113, 124	0
1	B	425/499 (85%)	-0.04	6 (1%) 75 63	35, 68, 104, 126	0
1	C	435/499 (87%)	0.03	13 (2%) 51 35	39, 82, 118, 132	0
All	All	1285/1497 (85%)	-0.01	23 (1%) 69 55	31, 73, 111, 132	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	403	SER	6.1
1	C	484	GLU	3.8
1	C	92	THR	3.8
1	C	482	SER	3.3
1	A	232	THR	2.9
1	C	481	MET	2.9
1	C	483	ASN	2.9
1	B	366	ALA	2.6
1	B	428	ALA	2.4
1	C	109	ILE	2.4
1	C	110	LEU	2.4
1	C	402	SER	2.4
1	C	105	ARG	2.4
1	A	217	ILE	2.4
1	B	483	ASN	2.2
1	C	157	THR	2.2
1	C	111	TYR	2.2
1	B	244	GLU	2.2
1	B	245	SER	2.1
1	A	255	ASP	2.1
1	C	471	ALA	2.0
1	A	231	GLN	2.0
1	B	159	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.