Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 06:59 AM UTC

PDB ID	:	2Q06 / pdb_00002q06
Title	:	Crystal structure of Influenza A Virus H5N1 Nucleoprotein
Authors	:	Ng, A.K.L.; Zhang, H.; Tan, K.; Wang, J.; Shaw, P.C.
Deposited on	:	2007-05-21
Resolution	:	3.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

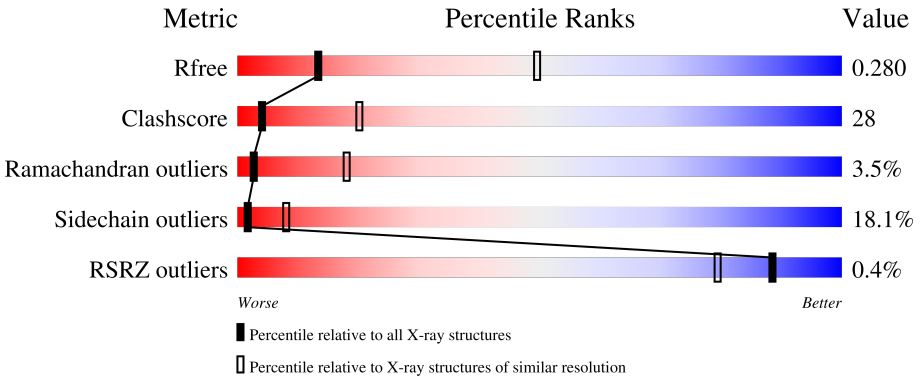
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

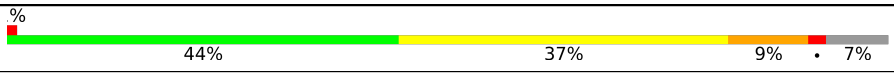
The reported resolution of this entry is 3.30 Å.

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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	504	
1	B	504	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7343 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3678	2269	696	686	27			
1	B	465	Total	C	N	O	S	0	0	0
			3665	2260	695	683	27			

There are 12 discrepancies between the modelled and reference sequences:

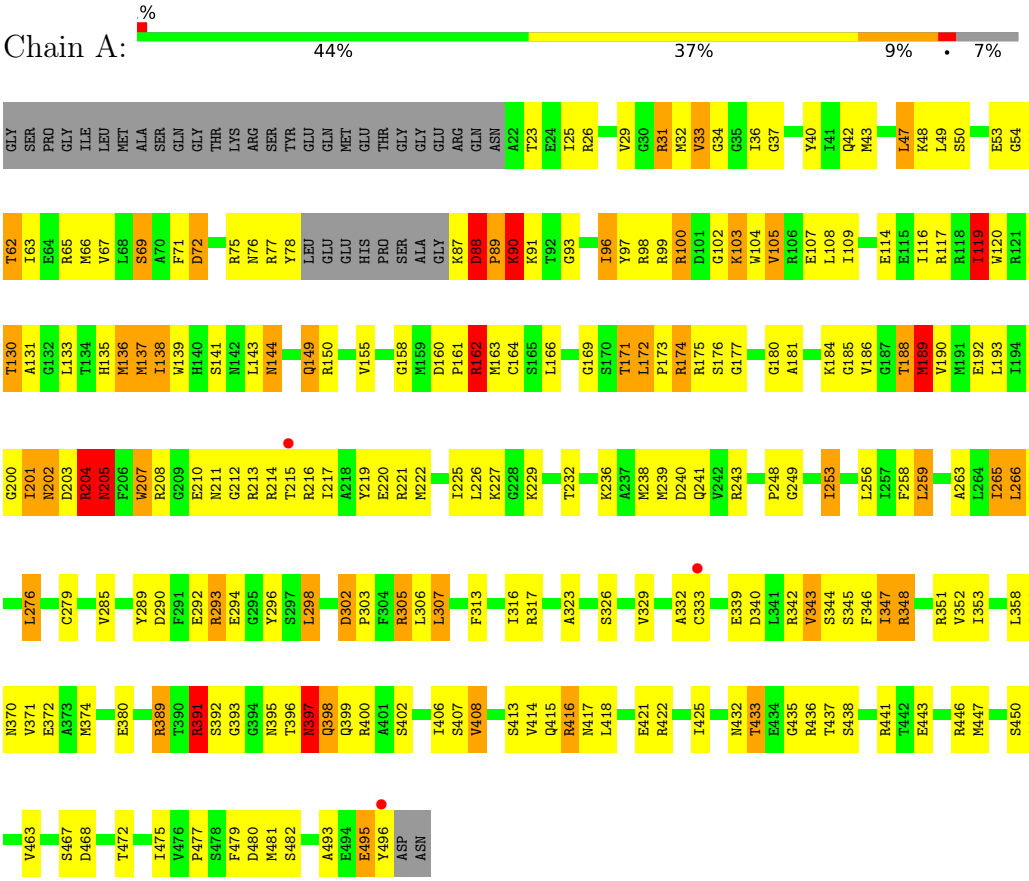
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9PX50
A	-4	SER	-	expression tag	UNP Q9PX50
A	-3	PRO	-	expression tag	UNP Q9PX50
A	-2	GLY	-	expression tag	UNP Q9PX50
A	-1	ILE	-	expression tag	UNP Q9PX50
A	0	LEU	-	expression tag	UNP Q9PX50
B	-5	GLY	-	expression tag	UNP Q9PX50
B	-4	SER	-	expression tag	UNP Q9PX50
B	-3	PRO	-	expression tag	UNP Q9PX50
B	-2	GLY	-	expression tag	UNP Q9PX50
B	-1	ILE	-	expression tag	UNP Q9PX50
B	0	LEU	-	expression tag	UNP Q9PX50

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

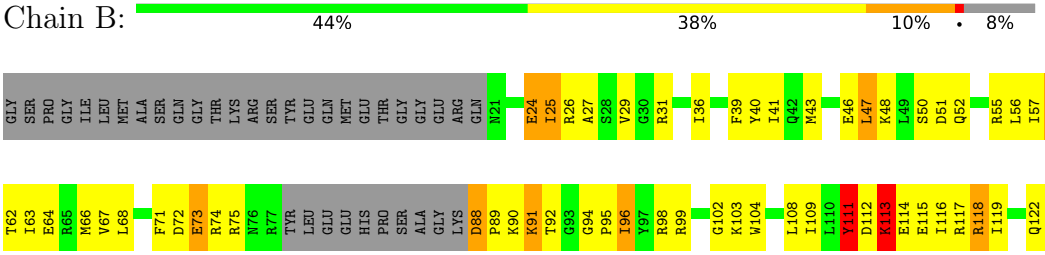
• Molecule 1: Nucleoprotein

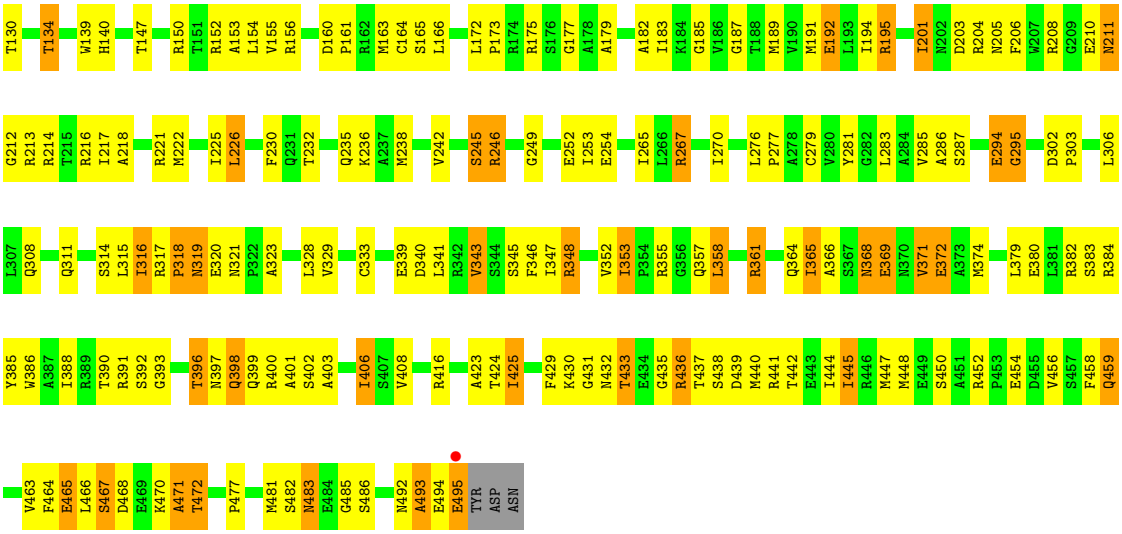
Chain A:



• Molecule 1: Nucleoprotein

Chain B:




T130 T134 W139 H140 T147 R150 T151 R152 A153 L154 V155 R156 D160 P161 R162 M163 C164 S165 L166 L172 P173 R174 R175 S176 G177 A178 A179 A182 I183 K184 G185 V186 G187 T188 M189 V190 M191 E192 L193 I194 R195 I201 N202 D203 R204 N205 F206 W207 R208 G209 E210 N211
G212 R213 R214 T215 R216 I217 A218 R221 M222 I225 L226 F230 Q231 T232 Q235 K236 A237 M238 V242 S245 R246 G249 E252 I253 E254 I265 L266 R267 I270 L276 P277 A278 C279 V280 Y281 G282 L283 A284 V285 A286 S287 E294 G295 D302 P303 L306
L307 Q308 Q311 S314 L315 I316 R317 P318 N319 E320 N321 P322 A323 L328 V329 C333 E339 D340 L341 R342 V343 S344 S345 F346 I347 R348 V352 I353 P354 R355 G356 Q357 L358 R361 Q364 I365 A366 S367 N368 E369 N370 V371 E372 A373 M374 L379 E380 L381 R382 S383 R384
Y385 W386 A387 I388 R389 T390 R391 S392 G393 T396 N397 Q398 Q399 R400 A401 S402 A403 I406 S407 V408 R416 A423 T424 I425 F429 K430 G431 N432 T433 E434 G435 R436 T437 S438 D439 M440 R441 T442 E443 I444 I445 R446 M447 M448 E449 S450 A451 R452 P453 E454 D455 V456 S457 F458 Q459
V463 F464 E465 L466 S467 D468 E469 K470 A471 T472 P477 M481 S482 N483 E484 G485 S486 N492 A493 E494 E496 TYR ASP ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	153.58Å 153.58Å 153.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 3.30 46.32 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.32-3.30) 99.7 (46.32-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.279 0.203 , 0.280	Depositor DCC
R_{free} test set	945 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	83.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 84.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.041 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7343	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.59	0/3737	0.99	11/5024 (0.2%)
1	B	0.59	0/3723	0.95	1/5003 (0.0%)
All	All	0.59	0/7460	0.97	12/10027 (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	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	ILE	CB-CA-C	-7.07	102.97	111.81
1	A	23	THR	N-CA-C	-7.06	104.41	113.16
1	B	403	ALA	N-CA-C	-6.26	104.91	113.30
1	A	391	ARG	N-CA-C	-5.69	105.01	112.41
1	A	189	MET	N-CA-C	5.42	117.61	111.11
1	A	353	ILE	CA-C-N	5.38	125.37	119.89
1	A	353	ILE	C-N-CA	5.38	125.37	119.89
1	A	347	ILE	CB-CA-C	-5.33	104.87	112.22
1	A	100	ARG	N-CA-C	5.30	117.45	108.02
1	A	418	LEU	CA-C-N	5.29	126.45	119.84
1	A	418	LEU	C-N-CA	5.29	126.45	119.84
1	A	138	ILE	CB-CA-C	-5.19	105.23	112.02

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	ARG	Sidechain
1	A	479	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3678	0	3639	197	0
1	B	3665	0	3639	212	0
All	All	7343	0	7278	405	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 28.

All (405) 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:B:398:GLN:HB3	1:B:447:MET:HE3	1.27	1.12
1:A:204:ARG:HE	1:A:204:ARG:HA	1.20	1.06
1:A:90:LYS:H	1:A:90:LYS:HD3	1.18	1.02
1:A:103:LYS:H	1:A:103:LYS:HD2	1.24	0.99
1:B:152:ARG:O	1:B:156:ARG:HG2	1.69	0.92
1:B:39:PHE:CZ	1:B:67:VAL:CG2	2.54	0.91
1:B:399:GLN:HE21	1:B:401:ALA:HB2	1.36	0.90
1:B:91:LYS:HB3	1:B:112:ASP:HA	1.54	0.90
1:A:433:THR:HG23	1:A:435:GLY:H	1.34	0.89
1:B:39:PHE:CZ	1:B:67:VAL:HG21	2.08	0.89
1:B:88:ASP:HB2	1:B:89:PRO:HD3	1.54	0.89
1:B:494:GLU:O	1:B:495:GLU:HG3	1.73	0.88
1:B:232:THR:OG1	1:B:235:GLN:HB2	1.74	0.86
1:B:124:ASN:H	1:B:124:ASN:HD22	1.19	0.85
1:B:317:ARG:HB3	1:B:318:PRO:HD2	1.57	0.84
1:A:340:ASP:OD1	1:A:342:ARG:HG3	1.76	0.84
1:B:124:ASN:HD22	1:B:124:ASN:N	1.76	0.83
1:B:314:SER:HB3	1:B:379:LEU:HD21	1.59	0.83
1:A:72:ASP:HB2	1:A:75:ARG:O	1.78	0.82
1:A:207:TRP:HA	1:A:212:GLY:HA2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PHE:CE2	1:B:67:VAL:HG21	2.18	0.79
1:B:315:LEU:HD13	1:B:374:MET:HE3	1.65	0.79
1:B:43:MET:HA	1:B:46:GLU:OE1	1.83	0.79
1:A:189:MET:O	1:A:193:LEU:HD12	1.84	0.78
1:B:160:ASP:H	1:B:163:MET:HE2	1.47	0.78
1:A:298:LEU:HD22	1:A:298:LEU:H	1.47	0.77
1:B:90:LYS:O	1:B:113:LYS:HD2	1.84	0.77
1:A:238:MET:HE3	1:A:259:LEU:HD13	1.64	0.76
1:A:213:ARG:O	1:A:217:ILE:HG12	1.86	0.76
1:A:65:ARG:O	1:A:69:SER:HB2	1.86	0.76
1:B:62:THR:HG22	1:B:66:MET:CE	2.17	0.75
1:B:192:GLU:HB3	1:B:222:MET:HE1	1.69	0.74
1:A:221:ARG:O	1:A:225:ILE:HG12	1.89	0.73
1:B:399:GLN:NE2	1:B:401:ALA:HB2	2.04	0.72
1:B:398:GLN:CB	1:B:447:MET:HE3	2.16	0.72
1:B:90:LYS:C	1:B:91:LYS:HG2	2.14	0.72
1:B:74:ARG:O	1:B:75:ARG:NH1	2.23	0.72
1:B:214:ARG:HB3	1:B:214:ARG:NH1	2.05	0.72
1:B:346:PHE:HE2	1:B:463:VAL:HG21	1.55	0.72
1:B:55:ARG:HH11	1:B:283:LEU:HD22	1.53	0.71
1:B:150:ARG:HD2	1:B:153:ALA:H	1.53	0.71
1:B:203:ASP:CG	1:B:204:ARG:N	2.47	0.71
1:A:208:ARG:HH11	1:A:208:ARG:HB3	1.52	0.71
1:B:465:GLU:OE2	1:B:466:LEU:N	2.23	0.71
1:A:163:MET:HB3	1:A:166:LEU:HD12	1.73	0.71
1:A:201:ILE:HG12	1:A:249:GLY:HA2	1.73	0.70
1:B:154:LEU:HD13	1:B:161:PRO:HA	1.72	0.70
1:B:55:ARG:NH2	1:B:311:GLN:HB3	2.06	0.70
1:A:185:GLY:HA2	1:A:270:ILE:HG21	1.73	0.70
1:A:62:THR:HG21	1:A:96:ILE:HG13	1.72	0.70
1:B:203:ASP:CG	1:B:204:ARG:H	1.98	0.70
1:B:294:GLU:CD	1:B:294:GLU:H	1.99	0.70
1:B:96:ILE:HD12	1:B:109:ILE:HG12	1.74	0.70
1:B:172:LEU:HD23	1:B:173:PRO:HD2	1.73	0.69
1:B:371:VAL:HB	1:B:374:MET:HE2	1.74	0.69
1:B:483:ASN:HB2	1:B:485:GLY:O	1.92	0.69
1:A:47:LEU:O	1:A:98:ARG:NH2	2.26	0.69
1:B:62:THR:HG22	1:B:66:MET:HE3	1.75	0.69
1:B:495:GLU:C	1:B:495:GLU:OE1	2.35	0.68
1:A:340:ASP:HB3	1:A:343:VAL:HG13	1.76	0.68
1:A:437:THR:O	1:A:441:ARG:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:H	1:A:103:LYS:CD	2.02	0.68
1:A:221:ARG:HH11	1:A:221:ARG:HB3	1.57	0.68
1:A:232:THR:O	1:A:236:LYS:HG3	1.94	0.68
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.09	0.66
1:A:238:MET:HE3	1:A:259:LEU:CD1	2.25	0.66
1:B:88:ASP:HB2	1:B:89:PRO:CD	2.22	0.66
1:A:204:ARG:HA	1:A:204:ARG:NE	2.01	0.66
1:A:348:ARG:NH2	1:A:380:GLU:O	2.28	0.66
1:B:71:PHE:CE2	1:B:117:ARG:HG3	2.31	0.66
1:B:191:MET:HE3	1:B:195:ARG:HH12	1.62	0.65
1:A:137:MET:O	1:A:137:MET:HG2	1.95	0.65
1:B:246:ARG:HA	1:B:246:ARG:HH11	1.62	0.65
1:B:39:PHE:HZ	1:B:67:VAL:CG2	2.06	0.65
1:A:143:LEU:HA	1:A:332:ALA:HB1	1.79	0.65
1:B:245:SER:HB2	1:B:436:ARG:HH12	1.61	0.65
1:A:42:GLN:HE22	1:B:319:ASN:HB2	1.61	0.64
1:A:90:LYS:HD3	1:A:90:LYS:N	2.03	0.64
1:B:75:ARG:HA	1:B:75:ARG:CZ	2.27	0.64
1:B:440:MET:O	1:B:444:ILE:HG12	1.98	0.64
1:A:103:LYS:HD2	1:A:103:LYS:N	2.04	0.64
1:A:31:ARG:NH2	1:A:127:GLU:OE1	2.31	0.64
1:A:129:ALA:O	1:A:131:ALA:N	2.31	0.64
1:B:399:GLN:O	1:B:400:ARG:HB3	1.98	0.63
1:B:361:ARG:O	1:B:361:ARG:HG3	1.98	0.63
1:B:386:TRP:NE1	1:B:464:PHE:HB2	2.14	0.62
1:B:72:ASP:O	1:B:73:GLU:HB3	1.99	0.62
1:B:154:LEU:CD1	1:B:161:PRO:HA	2.29	0.62
1:B:91:LYS:HA	1:B:113:LYS:H	1.62	0.62
1:A:184:LYS:HD3	1:A:189:MET:HE3	1.81	0.62
1:A:26:ARG:NH2	1:A:302:ASP:OD1	2.33	0.62
1:A:317:ARG:HG2	1:A:374:MET:HE2	1.81	0.62
1:B:399:GLN:HG3	1:B:401:ALA:H	1.64	0.62
1:B:115:GLU:O	1:B:119:ILE:HG13	2.00	0.62
1:A:93:GLY:HA3	1:A:109:ILE:O	2.00	0.61
1:A:207:TRP:CZ2	1:A:248:PRO:HD2	2.35	0.61
1:B:90:LYS:O	1:B:91:LYS:HG2	2.00	0.61
1:A:160:ASP:CG	1:A:162:ARG:HB2	2.26	0.61
1:B:88:ASP:CB	1:B:89:PRO:HD3	2.28	0.61
1:A:197:ILE:HG21	1:A:253:ILE:HG22	1.82	0.61
1:B:281:TYR:O	1:B:285:VAL:HG23	2.01	0.61
1:A:29:VAL:HG12	1:A:296:TYR:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:O	1:A:229:LYS:NZ	2.31	0.60
1:A:406:ILE:HG21	1:A:425:ILE:HD11	1.84	0.60
1:A:204:ARG:HE	1:A:204:ARG:CA	2.04	0.60
1:A:99:ARG:NH1	1:A:102:GLY:O	2.34	0.60
1:A:36:ILE:HD12	1:A:136:MET:HE2	1.83	0.60
1:A:395:ASN:O	1:A:396:THR:HG23	2.01	0.60
1:B:124:ASN:N	1:B:124:ASN:ND2	2.47	0.59
1:A:155:VAL:O	1:A:158:GLY:N	2.34	0.59
1:A:370:ASN:ND2	1:A:372:GLU:HB3	2.17	0.59
1:B:466:LEU:C	1:B:468:ASP:H	2.11	0.59
1:A:175:ARG:O	1:A:175:ARG:HG3	2.02	0.59
1:B:276:LEU:N	1:B:276:LEU:HD12	2.18	0.59
1:A:290:ASP:O	1:A:294:GLU:HG2	2.02	0.59
1:B:353:ILE:HD11	1:B:358:LEU:HD12	1.84	0.59
1:A:292:GLU:HB2	1:B:368:ASN:CG	2.28	0.58
1:B:346:PHE:CZ	1:B:477:PRO:HB3	2.38	0.58
1:A:205:ASN:HB2	1:A:208:ARG:HD2	1.85	0.58
1:B:213:ARG:O	1:B:216:ARG:HB3	2.03	0.58
1:B:429:PHE:HA	1:B:432:ASN:HD21	1.68	0.58
1:B:26:ARG:NH1	1:B:294:GLU:O	2.37	0.58
1:A:177:GLY:O	1:A:180:GLY:N	2.35	0.58
1:B:483:ASN:C	1:B:485:GLY:H	2.11	0.58
1:A:210:GLU:HG3	1:A:211:ASN:H	1.69	0.58
1:B:39:PHE:CZ	1:B:67:VAL:HG22	2.39	0.58
1:B:124:ASN:H	1:B:124:ASN:ND2	1.96	0.58
1:B:494:GLU:HG3	1:B:495:GLU:H	1.68	0.58
1:A:89:PRO:HB2	1:A:90:LYS:HD3	1.85	0.58
1:B:346:PHE:CE1	1:B:477:PRO:HB3	2.39	0.58
1:A:421:GLU:O	1:A:425:ILE:HG12	2.04	0.57
1:B:492:ASN:O	1:B:493:ALA:HB2	2.03	0.57
1:B:214:ARG:CB	1:B:214:ARG:HH11	2.18	0.57
1:B:495:GLU:OE1	1:B:495:GLU:O	2.22	0.57
1:A:190:VAL:HG13	1:A:256:LEU:HB3	1.86	0.57
1:A:238:MET:HG3	1:A:238:MET:O	2.05	0.57
1:B:26:ARG:HG3	1:B:295:GLY:HA3	1.86	0.57
1:B:316:ILE:HG23	1:B:320:GLU:HB2	1.86	0.57
1:B:62:THR:HG23	1:B:95:PRO:HD2	1.86	0.57
1:B:41:ILE:HD13	1:B:286:ALA:HB2	1.86	0.56
1:B:60:SER:O	1:B:64:GLU:HG3	2.05	0.56
1:A:196:MET:HE1	1:A:219:TYR:HB2	1.87	0.56
1:B:214:ARG:NH1	1:B:214:ARG:CB	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:HE	1:A:220:GLU:CG	2.18	0.56
1:B:185:GLY:HA2	1:B:270:ILE:HD12	1.87	0.56
1:A:414:VAL:O	1:A:416:ARG:HG3	2.05	0.56
1:A:199:ARG:HA	1:A:199:ARG:HH11	1.70	0.56
1:B:371:VAL:HA	1:B:374:MET:HG3	1.87	0.56
1:B:139:TRP:CD1	1:B:140:HIS:HD2	2.23	0.56
1:B:217:ILE:HG13	1:B:218:ALA:N	2.15	0.56
1:B:104:TRP:O	1:B:371:VAL:HG22	2.06	0.55
1:B:430:LYS:HB3	1:B:445:ILE:HG21	1.88	0.55
1:B:24:GLU:OE1	1:B:25:ILE:HG22	2.07	0.55
1:A:276:LEU:HD22	1:A:307:LEU:HD21	1.87	0.55
1:A:371:VAL:HG12	1:A:371:VAL:O	2.06	0.55
1:B:57:ILE:O	1:B:61:ILE:HG12	2.06	0.55
1:A:172:LEU:HD12	1:A:173:PRO:HD2	1.88	0.55
1:B:317:ARG:HB2	1:B:320:GLU:OE2	2.06	0.55
1:B:396:THR:O	1:B:396:THR:HG22	2.06	0.55
1:A:128:ASP:O	1:A:129:ALA:C	2.50	0.54
1:A:181:ALA:HA	1:A:184:LYS:HD2	1.89	0.54
1:B:147:THR:HG22	1:B:328:LEU:HD21	1.89	0.54
1:A:76:ASN:O	1:A:173:PRO:HG3	2.07	0.54
1:A:226:LEU:HB3	1:A:239:MET:HE2	1.88	0.54
1:B:57:ILE:HG23	1:B:58:GLN:N	2.22	0.54
1:B:139:TRP:CZ2	1:B:277:PRO:HG3	2.43	0.54
1:B:294:GLU:CD	1:B:294:GLU:N	2.63	0.54
1:A:406:ILE:O	1:A:406:ILE:CG2	2.55	0.54
1:B:194:ILE:HG12	1:B:253:ILE:HG23	1.89	0.53
1:B:431:GLY:HA3	1:B:442:THR:HA	1.90	0.53
1:A:144:ASN:OD1	1:A:150:ARG:NH2	2.41	0.53
1:B:238:MET:HB2	1:B:440:MET:CG	2.39	0.53
1:B:348:ARG:NH2	1:B:380:GLU:O	2.42	0.53
1:B:41:ILE:CD1	1:B:286:ALA:HB2	2.39	0.53
1:A:365:ILE:N	1:A:365:ILE:HD12	2.24	0.53
1:B:246:ARG:HH11	1:B:246:ARG:CA	2.22	0.53
1:A:107:GLU:O	1:A:108:LEU:C	2.52	0.52
1:B:321:ASN:ND2	1:B:323:ALA:H	2.07	0.52
1:B:118:ARG:O	1:B:122:GLN:HG2	2.10	0.52
1:B:470:LYS:O	1:B:472:THR:N	2.38	0.52
1:A:77:ARG:O	1:A:78:TYR:C	2.52	0.52
1:A:265:ILE:O	1:A:267:ARG:N	2.42	0.52
1:A:346:PHE:CE2	1:A:477:PRO:HB3	2.45	0.52
1:B:450:SER:HA	1:B:452:ARG:HH12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:OH	1:A:54:GLY:O	2.20	0.52
1:A:197:ILE:HG21	1:A:253:ILE:CG2	2.40	0.52
1:A:292:GLU:HB2	1:B:368:ASN:OD1	2.09	0.52
1:B:283:LEU:O	1:B:287:SER:HB2	2.09	0.52
1:A:143:LEU:HA	1:A:332:ALA:CB	2.39	0.52
1:B:317:ARG:HB2	1:B:320:GLU:CD	2.35	0.52
1:A:114:GLU:HB3	1:A:117:ARG:HH11	1.73	0.52
1:B:265:ILE:HG13	1:B:448:MET:HE3	1.89	0.52
1:A:289:TYR:CE1	1:A:294:GLU:HG3	2.45	0.51
1:B:437:THR:O	1:B:441:ARG:HG3	2.10	0.51
1:A:144:ASN:OD1	1:A:171:THR:HG21	2.09	0.51
1:A:89:PRO:C	1:A:91:LYS:H	2.17	0.51
1:A:266:LEU:HA	1:A:396:THR:CG2	2.40	0.51
1:B:41:ILE:C	1:B:43:MET:H	2.17	0.51
1:B:51:ASP:O	1:B:55:ARG:HD3	2.11	0.51
1:B:317:ARG:HD3	1:B:369:GLU:OE1	2.10	0.51
1:B:345:SER:HA	1:B:352:VAL:HG23	1.92	0.51
1:B:314:SER:HB2	1:B:379:LEU:HD11	1.93	0.51
1:B:433:THR:HG23	1:B:435:GLY:H	1.75	0.51
1:B:62:THR:O	1:B:66:MET:HB2	2.10	0.51
1:B:366:ALA:N	1:B:369:GLU:OE2	2.41	0.51
1:A:76:ASN:O	1:A:173:PRO:CB	2.59	0.51
1:B:134:THR:HG21	1:B:177:GLY:H	1.76	0.51
1:B:91:LYS:CB	1:B:112:ASP:HA	2.35	0.50
1:B:111:TYR:O	1:B:112:ASP:HB3	2.10	0.50
1:B:214:ARG:HB3	1:B:214:ARG:CZ	2.41	0.50
1:B:399:GLN:HE21	1:B:401:ALA:CB	2.16	0.50
1:B:46:GLU:H	1:B:46:GLU:CD	2.19	0.50
1:A:59:ASN:O	1:A:63:ILE:HG13	2.11	0.50
1:A:72:ASP:CB	1:A:75:ARG:O	2.56	0.50
1:A:193:LEU:HG	1:A:222:MET:HE2	1.94	0.50
1:A:433:THR:HG22	1:A:438:SER:HB2	1.94	0.50
1:B:72:ASP:OD2	1:B:74:ARG:HB2	2.12	0.50
1:A:75:ARG:NH1	1:A:175:ARG:HG2	2.27	0.50
1:B:317:ARG:HB3	1:B:318:PRO:CD	2.34	0.50
1:A:298:LEU:HD22	1:A:298:LEU:N	2.22	0.49
1:B:172:LEU:CD2	1:B:173:PRO:HD2	2.42	0.49
1:A:116:ILE:HD13	1:A:116:ILE:N	2.26	0.49
1:B:66:MET:HE1	1:B:109:ILE:HD11	1.95	0.49
1:A:40:TYR:CE2	1:A:279:CYS:HA	2.47	0.49
1:A:130:THR:HG22	1:A:133:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ILE:O	1:B:391:ARG:HA	2.13	0.49
1:B:62:THR:HG22	1:B:66:MET:HE1	1.92	0.49
1:B:43:MET:HG2	1:B:63:ILE:HD12	1.95	0.49
1:B:72:ASP:OD2	1:B:175:ARG:NH1	2.45	0.49
1:A:161:PRO:C	1:A:163:MET:H	2.21	0.48
1:B:56:LEU:HD21	1:B:315:LEU:HG	1.95	0.48
1:A:129:ALA:C	1:A:131:ALA:H	2.21	0.48
1:A:201:ILE:CG1	1:A:249:GLY:HA2	2.43	0.48
1:B:55:ARG:NH1	1:B:283:LEU:HD13	2.28	0.48
1:B:152:ARG:HA	1:B:155:VAL:HG22	1.95	0.48
1:B:483:ASN:C	1:B:485:GLY:N	2.71	0.48
1:A:344:SER:O	1:A:348:ARG:HB2	2.14	0.48
1:A:76:ASN:O	1:A:173:PRO:HB3	2.14	0.48
1:B:95:PRO:O	1:B:96:ILE:HG13	2.14	0.48
1:B:464:PHE:CE2	1:B:471:ALA:HB1	2.49	0.48
1:B:317:ARG:O	1:B:318:PRO:C	2.56	0.48
1:B:339:GLU:CD	1:B:343:VAL:HG11	2.39	0.48
1:A:119:ILE:O	1:A:120:TRP:C	2.56	0.48
1:A:463:VAL:HG22	1:A:475:ILE:HB	1.95	0.48
1:B:56:LEU:HG	1:B:58:GLN:HG2	1.95	0.48
1:A:406:ILE:CG2	1:A:425:ILE:HD11	2.43	0.48
1:A:451:ALA:O	1:A:452:ARG:HD3	2.14	0.48
1:B:429:PHE:HA	1:B:432:ASN:ND2	2.29	0.48
1:A:240:ASP:OD2	1:A:243:ARG:NH2	2.46	0.47
1:A:302:ASP:HA	1:A:305:ARG:NH1	2.29	0.47
1:A:71:PHE:CZ	1:A:117:ARG:HG2	2.49	0.47
1:B:238:MET:HB2	1:B:440:MET:HG2	1.97	0.47
1:B:353:ILE:HD11	1:B:358:LEU:CD1	2.43	0.47
1:A:259:LEU:HD12	1:A:259:LEU:HA	1.76	0.47
1:B:27:ALA:O	1:B:31:ARG:N	2.48	0.47
1:B:386:TRP:NE1	1:B:464:PHE:CB	2.77	0.47
1:A:50:SER:HB3	1:A:53:GLU:CG	2.45	0.47
1:A:407:SER:OG	1:A:408:VAL:N	2.47	0.47
1:B:191:MET:CE	1:B:195:ARG:HH12	2.24	0.47
1:B:371:VAL:O	1:B:372:GLU:HB2	2.15	0.47
1:A:90:LYS:H	1:A:90:LYS:CD	2.01	0.47
1:A:216:ARG:HE	1:A:220:GLU:HG3	1.79	0.47
1:A:26:ARG:NH1	1:A:294:GLU:O	2.47	0.47
1:A:450:SER:O	1:A:452:ARG:NH1	2.47	0.47
1:B:62:THR:HG21	1:B:95:PRO:O	2.15	0.47
1:B:302:ASP:HB2	1:B:303:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HA	1:A:396:THR:HG21	1.95	0.47
1:B:386:TRP:CE2	1:B:464:PHE:HB2	2.50	0.47
1:A:199:ARG:O	1:A:203:ASP:HB3	2.14	0.47
1:A:226:LEU:HD23	1:A:226:LEU:O	2.14	0.46
1:A:198:LYS:C	1:A:200:GLY:N	2.73	0.46
1:A:329:VAL:O	1:A:333:CYS:SG	2.72	0.46
1:A:186:VAL:O	1:A:190:VAL:HG23	2.16	0.46
1:B:47:LEU:O	1:B:98:ARG:NH2	2.39	0.46
1:A:339:GLU:OE1	1:A:340:ASP:N	2.49	0.46
1:A:104:TRP:HB2	1:A:371:VAL:HG12	1.97	0.45
1:B:88:ASP:CB	1:B:89:PRO:CD	2.90	0.45
1:B:118:ARG:NH2	1:B:122:GLN:HG3	2.31	0.45
1:A:129:ALA:C	1:A:131:ALA:N	2.74	0.45
1:B:189:MET:HE2	1:B:189:MET:HB3	1.80	0.45
1:B:203:ASP:OD2	1:B:206:PHE:N	2.48	0.45
1:A:29:VAL:O	1:A:32:MET:HG3	2.17	0.45
1:A:276:LEU:N	1:A:276:LEU:HD23	2.32	0.45
1:A:323:ALA:O	1:A:326:SER:HB2	2.17	0.45
1:A:391:ARG:HE	1:A:391:ARG:HB3	1.58	0.45
1:B:221:ARG:O	1:B:225:ILE:HG12	2.16	0.45
1:B:329:VAL:HG12	1:B:333:CYS:SG	2.56	0.45
1:A:406:ILE:HG23	1:A:421:GLU:HB2	1.99	0.45
1:A:226:LEU:HD23	1:A:226:LEU:C	2.42	0.45
1:A:175:ARG:O	1:A:175:ARG:CG	2.65	0.45
1:A:467:SER:HA	1:B:156:ARG:HH22	1.81	0.45
1:B:214:ARG:HH11	1:B:214:ARG:HB2	1.81	0.45
1:B:365:ILE:HG12	1:B:374:MET:HE1	1.99	0.45
1:B:406:ILE:HG23	1:B:425:ILE:HD11	1.99	0.45
1:B:438:SER:O	1:B:441:ARG:HB2	2.17	0.45
1:A:136:MET:HE3	1:A:136:MET:HB2	1.64	0.44
1:B:55:ARG:HH21	1:B:311:GLN:HE21	1.65	0.44
1:A:50:SER:HB3	1:A:53:GLU:CD	2.42	0.44
1:A:161:PRO:C	1:A:163:MET:N	2.75	0.44
1:A:392:SER:OG	1:A:393:GLY:N	2.50	0.44
1:A:397:ASN:HB2	1:A:398:GLN:H	1.55	0.44
1:B:73:GLU:O	1:B:73:GLU:CG	2.66	0.44
1:A:263:ALA:HA	1:A:266:LEU:O	2.16	0.44
1:A:495:GLU:O	1:A:496:TYR:HB2	2.17	0.44
1:B:40:TYR:CE2	1:B:279:CYS:HA	2.53	0.44
1:B:114:GLU:HB2	1:B:117:ARG:NH1	2.32	0.44
1:A:137:MET:HE3	1:A:172:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HB2	1:A:49:LEU:HG	1.99	0.44
1:A:211:ASN:HA	1:A:214:ARG:HB2	1.99	0.44
1:A:221:ARG:HH11	1:A:221:ARG:CB	2.28	0.44
1:A:289:TYR:CZ	1:A:294:GLU:HG3	2.53	0.44
1:A:62:THR:HG21	1:A:96:ILE:CG1	2.45	0.44
1:A:169:GLY:O	1:A:172:LEU:HB2	2.16	0.44
1:B:116:ILE:HA	1:B:119:ILE:HD12	1.99	0.44
1:A:298:LEU:H	1:A:298:LEU:CD2	2.26	0.44
1:A:75:ARG:HB2	1:A:174:ARG:O	2.18	0.44
1:A:433:THR:HG22	1:A:438:SER:CA	2.48	0.44
1:A:351:ARG:HH21	1:A:496:TYR:C	2.26	0.44
1:B:216:ARG:NH1	1:B:246:ARG:NH1	2.66	0.44
1:B:317:ARG:CB	1:B:318:PRO:CD	2.93	0.44
1:B:75:ARG:NH2	1:B:90:LYS:NZ	2.66	0.43
1:A:55:ARG:HD2	1:A:313:PHE:CE1	2.53	0.43
1:A:397:ASN:HA	1:A:447:MET:CE	2.48	0.43
1:B:61:ILE:HA	1:B:64:GLU:OE1	2.18	0.43
1:B:123:ALA:O	1:B:125:ASN:N	2.51	0.43
1:B:210:GLU:C	1:B:212:GLY:N	2.76	0.43
1:A:37:GLY:HA3	1:A:285:VAL:HG21	1.99	0.43
1:B:166:LEU:HB3	1:B:187:GLY:H	1.84	0.43
1:B:205:ASN:HA	1:B:208:ARG:HG2	1.99	0.43
1:B:339:GLU:OE1	1:B:340:ASP:N	2.50	0.43
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.64	0.43
1:A:192:GLU:O	1:A:195:ARG:HB3	2.19	0.43
1:A:135:HIS:O	1:A:138:ILE:HB	2.18	0.43
1:B:55:ARG:HG2	1:B:283:LEU:HD11	1.99	0.43
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.87	0.43
1:B:458:PHE:O	1:B:459:GLN:C	2.62	0.43
1:A:76:ASN:HB3	1:A:77:ARG:H	1.58	0.43
1:B:254:GLU:OE2	1:B:254:GLU:HA	2.19	0.43
1:A:43:MET:HE1	1:A:116:ILE:HD12	1.99	0.43
1:B:73:GLU:O	1:B:73:GLU:HG2	2.18	0.43
1:B:492:ASN:O	1:B:493:ALA:CB	2.65	0.43
1:A:188:THR:HG22	1:A:189:MET:N	2.33	0.43
1:B:308:GLN:HA	1:B:382:ARG:HG2	2.01	0.43
1:A:149:GLN:HE21	1:A:149:GLN:HA	1.84	0.43
1:A:221:ARG:CB	1:A:221:ARG:NH1	2.82	0.43
1:A:345:SER:HA	1:A:352:VAL:HG23	2.01	0.43
1:B:238:MET:O	1:B:242:VAL:HG23	2.19	0.43
1:A:58:GLN:HE21	1:A:58:GLN:HB3	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:MET:HG2	1:B:116:ILE:HD13	2.01	0.42
1:B:355:ARG:C	1:B:357:GLN:H	2.25	0.42
1:A:433:THR:HG23	1:A:435:GLY:N	2.17	0.42
1:A:87:LYS:O	1:A:88:ASP:CB	2.67	0.42
1:A:422:ARG:HG2	1:A:422:ARG:HH11	1.84	0.42
1:B:160:ASP:OD1	1:B:161:PRO:HD2	2.20	0.42
1:A:88:ASP:OD1	1:A:88:ASP:C	2.61	0.42
1:A:97:TYR:HA	1:A:105:VAL:O	2.19	0.42
1:A:141:SER:HB2	1:A:172:LEU:HD13	2.00	0.42
1:A:298:LEU:N	1:A:298:LEU:HD13	2.34	0.42
1:B:94:GLY:C	1:B:108:LEU:HD23	2.44	0.42
1:B:210:GLU:O	1:B:213:ARG:HB2	2.19	0.42
1:A:36:ILE:H	1:A:36:ILE:HG12	1.63	0.42
1:A:443:GLU:OE1	1:A:446:ARG:NH1	2.53	0.42
1:B:58:GLN:HG2	1:B:58:GLN:H	1.49	0.42
1:B:75:ARG:HA	1:B:75:ARG:NE	2.34	0.42
1:B:160:ASP:N	1:B:163:MET:HE2	2.26	0.42
1:A:406:ILE:O	1:A:406:ILE:HG22	2.20	0.42
1:B:57:ILE:CG2	1:B:58:GLN:N	2.81	0.42
1:B:267:ARG:HG3	1:B:393:GLY:O	2.19	0.42
1:A:417:ASN:HD22	1:A:417:ASN:H	1.66	0.42
1:A:433:THR:HG22	1:A:438:SER:HA	2.01	0.42
1:B:341:LEU:HD22	1:B:352:VAL:O	2.20	0.42
1:B:51:ASP:O	1:B:55:ARG:CD	2.68	0.42
1:B:112:ASP:O	1:B:114:GLU:N	2.53	0.42
1:B:211:ASN:C	1:B:211:ASN:HD22	2.28	0.42
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.54	0.42
1:A:143:LEU:HD12	1:A:143:LEU:O	2.20	0.41
1:B:99:ARG:HG2	1:B:102:GLY:O	2.20	0.41
1:B:124:ASN:O	1:B:125:ASN:C	2.62	0.41
1:A:75:ARG:HH11	1:A:175:ARG:HG2	1.85	0.41
1:B:390:THR:HB	1:B:392:SER:H	1.84	0.41
1:B:482:SER:O	1:B:483:ASN:C	2.63	0.41
1:A:290:ASP:CG	1:A:293:ARG:HB2	2.44	0.41
1:A:33:VAL:HG12	1:A:34:GLY:N	2.35	0.41
1:A:66:MET:HE2	1:A:66:MET:HB3	1.87	0.41
1:A:141:SER:OG	1:A:169:GLY:HA2	2.20	0.41
1:A:197:ILE:H	1:A:197:ILE:HG12	1.69	0.41
1:A:227:LYS:O	1:A:236:LYS:HE3	2.20	0.41
1:A:229:LYS:HD3	1:A:270:ILE:HG22	2.03	0.41
1:A:303:PRO:HG2	1:A:389:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASN:O	1:A:398:GLN:HB2	2.20	0.41
1:A:399:GLN:HE21	1:A:399:GLN:HB2	1.59	0.41
1:A:432:ASN:N	1:A:432:ASN:HD22	2.19	0.41
1:B:347:ILE:HA	1:B:385:TYR:HB2	2.02	0.41
1:A:100:ARG:NH1	1:A:107:GLU:OE2	2.54	0.40
1:B:226:LEU:HD22	1:B:230:PHE:CE1	2.56	0.40
1:B:267:ARG:H	1:B:267:ARG:HG2	1.71	0.40
1:A:258:PHE:CD2	1:A:258:PHE:C	2.98	0.40
1:B:179:ALA:O	1:B:182:ALA:HB3	2.22	0.40
1:A:119:ILE:H	1:A:119:ILE:HG12	1.52	0.40
1:B:201:ILE:HD11	1:B:249:GLY:HA2	2.04	0.40
1:A:195:ARG:HA	1:A:195:ARG:HD3	2.00	0.40
1:A:463:VAL:CG2	1:A:475:ILE:HB	2.51	0.40
1:B:321:ASN:ND2	1:B:321:ASN:C	2.77	0.40
1:A:202:ASN:HD22	1:A:202:ASN:HA	1.54	0.40
1:A:207:TRP:CZ2	1:A:248:PRO:CD	3.05	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	463/504 (92%)	389 (84%)	58 (12%)	16 (4%)	3	18
1	B	461/504 (92%)	389 (84%)	56 (12%)	16 (4%)	3	18
All	All	924/1008 (92%)	778 (84%)	114 (12%)	32 (4%)	3	18

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	A	493	ALA

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Mol	Chain	Res	Type
1	B	372	GLU
1	A	88	ASP
1	A	89	PRO
1	A	130	THR
1	A	162	ARG
1	A	204	ARG
1	A	205	ASN
1	A	266	LEU
1	A	468	ASP
1	B	467	SER
1	B	471	ALA
1	A	48	LYS
1	A	90	LYS
1	A	397	ASN
1	B	111	TYR
1	B	124	ASN
1	B	125	ASN
1	B	245	SER
1	B	486	SER
1	B	493	ALA
1	B	295	GLY
1	B	318	PRO
1	B	483	ASN
1	B	195	ARG
1	B	402	SER
1	B	423	ALA
1	A	453	PRO
1	B	113	LYS
1	A	201	ILE
1	A	265	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	387/420 (92%)	316 (82%)	71 (18%)	2 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	387/420 (92%)	318 (82%)	69 (18%)	2 8
All	All	774/840 (92%)	634 (82%)	140 (18%)	2 8

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	33	VAL
1	A	47	LEU
1	A	58	GLN
1	A	62	THR
1	A	67	VAL
1	A	69	SER
1	A	72	ASP
1	A	88	ASP
1	A	90	LYS
1	A	96	ILE
1	A	103	LYS
1	A	105	VAL
1	A	119	ILE
1	A	122	GLN
1	A	136	MET
1	A	137	MET
1	A	139	TRP
1	A	144	ASN
1	A	149	GLN
1	A	162	ARG
1	A	164	CYS
1	A	171	THR
1	A	172	LEU
1	A	174	ARG
1	A	176	SER
1	A	188	THR
1	A	189	MET
1	A	197	ILE
1	A	199	ARG
1	A	202	ASN
1	A	204	ARG
1	A	205	ASN
1	A	207	TRP
1	A	215	THR
1	A	241	GLN

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Mol	Chain	Res	Type
1	A	253	ILE
1	A	259	LEU
1	A	270	ILE
1	A	273	LYS
1	A	276	LEU
1	A	293	ARG
1	A	298	LEU
1	A	302	ASP
1	A	305	ARG
1	A	306	LEU
1	A	307	LEU
1	A	316	ILE
1	A	343	VAL
1	A	347	ILE
1	A	348	ARG
1	A	358	LEU
1	A	359	SER
1	A	364	GLN
1	A	389	ARG
1	A	391	ARG
1	A	397	ASN
1	A	400	ARG
1	A	402	SER
1	A	408	VAL
1	A	413	SER
1	A	415	GLN
1	A	416	ARG
1	A	433	THR
1	A	436	ARG
1	A	459	GLN
1	A	472	THR
1	A	480	ASP
1	A	481	MET
1	A	482	SER
1	A	495	GLU
1	B	24	GLU
1	B	25	ILE
1	B	29	VAL
1	B	36	ILE
1	B	47	LEU
1	B	48	LYS
1	B	50	SER

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Mol	Chain	Res	Type
1	B	52	GLN
1	B	58	GLN
1	B	73	GLU
1	B	88	ASP
1	B	91	LYS
1	B	92	THR
1	B	96	ILE
1	B	103	LYS
1	B	111	TYR
1	B	113	LYS
1	B	118	ARG
1	B	124	ASN
1	B	130	THR
1	B	134	THR
1	B	164	CYS
1	B	165	SER
1	B	183	ILE
1	B	192	GLU
1	B	201	ILE
1	B	211	ASN
1	B	226	LEU
1	B	236	LYS
1	B	246	ARG
1	B	252	GLU
1	B	267	ARG
1	B	294	GLU
1	B	306	LEU
1	B	316	ILE
1	B	319	ASN
1	B	343	VAL
1	B	348	ARG
1	B	353	ILE
1	B	358	LEU
1	B	361	ARG
1	B	364	GLN
1	B	365	ILE
1	B	368	ASN
1	B	369	GLU
1	B	371	VAL
1	B	383	SER
1	B	384	ARG
1	B	388	ILE

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Mol	Chain	Res	Type
1	B	396	THR
1	B	397	ASN
1	B	398	GLN
1	B	406	ILE
1	B	408	VAL
1	B	416	ARG
1	B	424	THR
1	B	425	ILE
1	B	433	THR
1	B	436	ARG
1	B	439	ASP
1	B	445	ILE
1	B	454	GLU
1	B	456	VAL
1	B	459	GLN
1	B	465	GLU
1	B	467	SER
1	B	472	THR
1	B	481	MET
1	B	495	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	122	GLN
1	A	142	ASN
1	A	149	GLN
1	A	202	ASN
1	A	247	ASN
1	A	309	ASN
1	A	311	GLN
1	A	334	HIS
1	A	368	ASN
1	A	405	GLN
1	A	409	GLN
1	A	417	ASN
1	A	432	ASN
1	B	52	GLN
1	B	124	ASN
1	B	140	HIS
1	B	211	ASN

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Mol	Chain	Res	Type
1	B	241	GLN
1	B	309	ASN
1	B	311	GLN
1	B	319	ASN
1	B	324	HIS
1	B	334	HIS
1	B	368	ASN
1	B	398	GLN
1	B	399	GLN
1	B	409	GLN
1	B	415	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 oligosaccharides 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^{th} 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^2)	Q<0.9
1	A	467/504 (92%)	-0.11	3 (0%)	85	73	30, 93, 109, 119	0
1	B	465/504 (92%)	-0.16	1 (0%)	91	86	73, 92, 106, 116	0
All	All	932/1008 (92%)	-0.14	4 (0%)	88	79	30, 93, 109, 119	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	CYS	4.1
1	A	496	TYR	2.3
1	A	215	THR	2.1
1	B	495	GLU	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.