Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:14 AM GMT

PDB ID	:	2G96
Title	:	Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase In Complex with Niconamide Mononucleotide
Authors	:	Eom, S.H.; Kim, M.-K.
Deposited on	:	2006-03-05
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

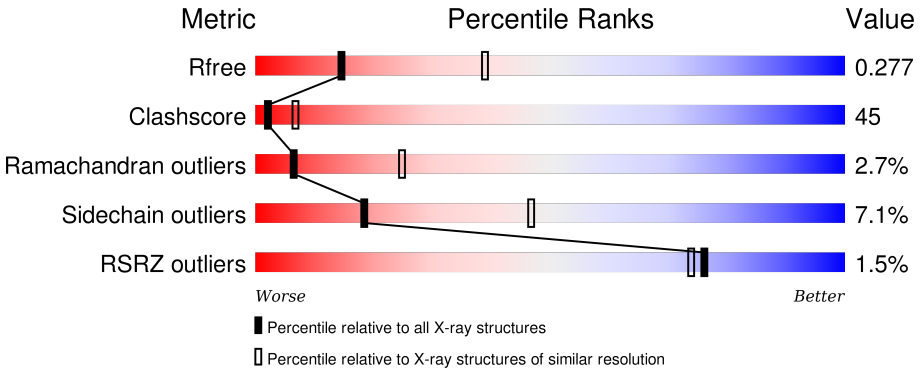
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 >=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 <=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	491	31% 56% 6% 6%
1	B	491	2% 34% 53% 7% 6%

2 Entry composition

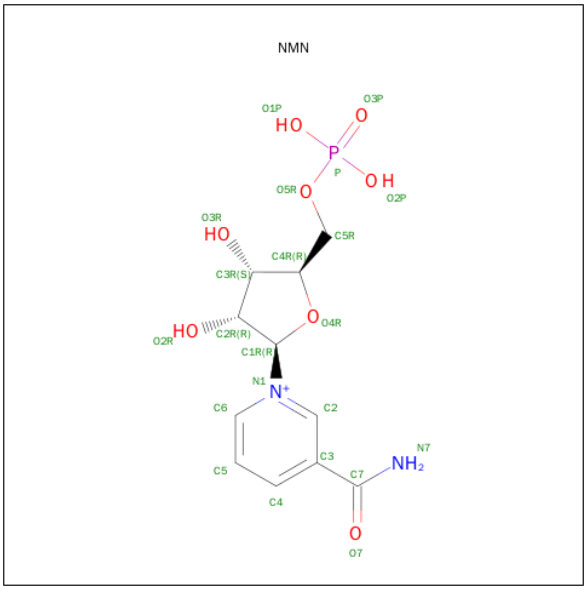
There are 3 unique types of molecules in this entry. The entry contains 7576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			
1	B	463	Total	C	N	O	S	0	0	0
			3700	2374	616	704	6			

- Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (three-letter code: NMN) (formula: $C_{11}H_{16}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 3 is water.

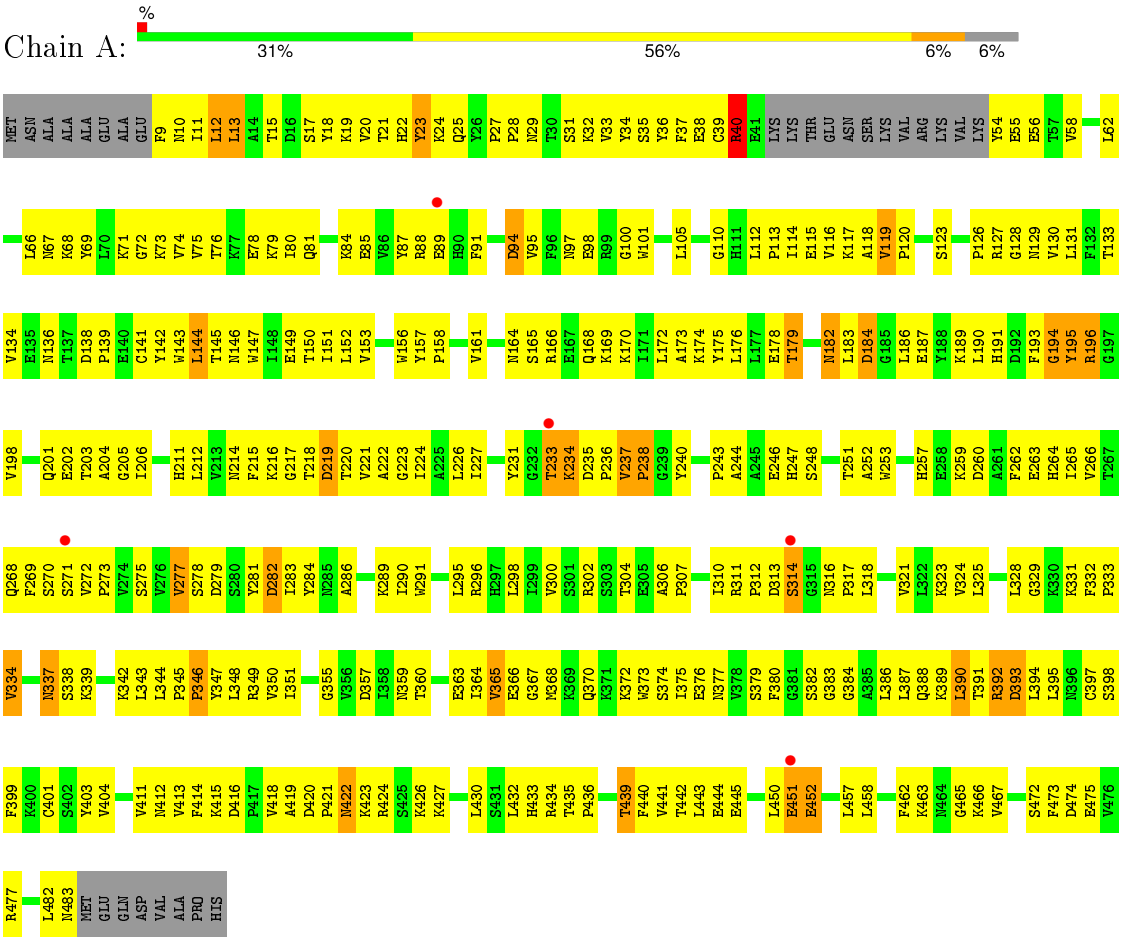
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	B	50	Total O 50 50	0	0

3 Residue-property plots (i)

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.

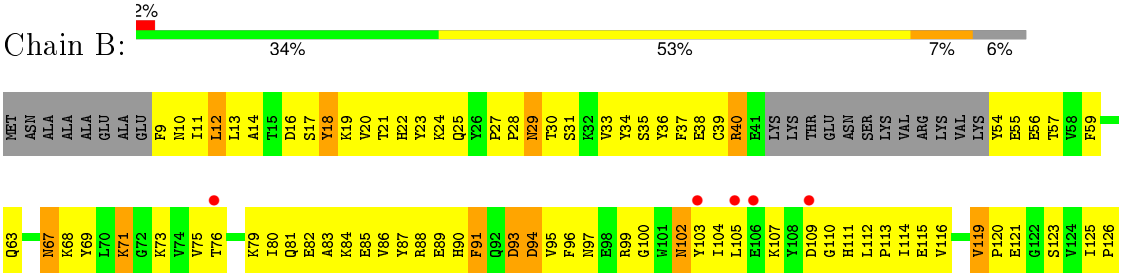
- Molecule 1: Nicotinamide phosphoribosyltransferase

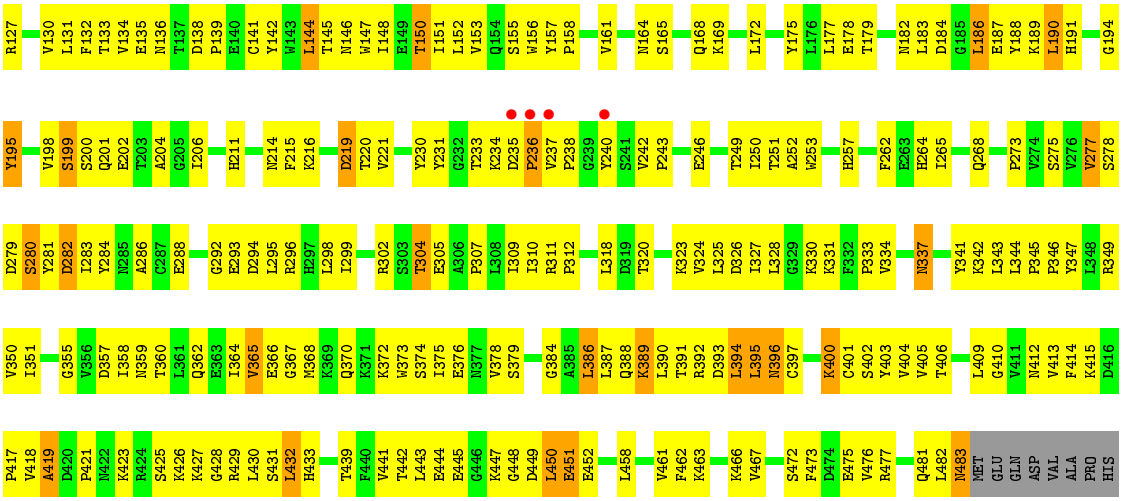
Chain A:



- Molecule 1: Nicotinamide phosphoribosyltransferase

Chain B:




R127 V130 L131 F132 T133 V134 E135 N136 T137 D138 P139 E140 C141 Y142 W143 L144 T145 N146 W147 I148 E149 T150 I151 L152 V153 Q154 S155 W156 Y157 P158 V161 N164 S165 Q168 K169 L172 Y175 L176 L177 E178 T179 N182 L183 D184 G185 L186 E187 Y188 K189 L190 H191 G194
Y195 V198 S199 S200 Q201 E202 T203 A204 G205 I206 H211 N214 F215 K216 D219 T220 V221 Y230 Y231 G232 T233 K234 D235 P236 V237 P238 G239 Y240 S241 V242 P243 E246 T249 I250 T251 A252 W253 H257 F262 E263 H264 I265 Q268 P273 V274 S275 V276 V277 S278
D279 S280 Y281 D282 I283 Y284 N285 A286 C287 E288 G292 E293 D294 L295 R296 H297 L298 I299 R302 S303 T304 E305 A306 P307 I308 I309 I310 R311 P312 L318 D319 T320 K323 V324 L325 D326 I327 L328 G329 K330 K331 F332 P333 V334 N337 Y341 K342 L343 L344 P345 P346 Y347 L348 R349
V350 I351 G355 V356 D357 I358 N359 T360 L361 Q362 E363 I364 V365 E366 G367 M368 K369 Q370 K371 K372 W373 S374 I375 E376 N377 V378 S379 G384 A385 L386 L387 Q388 K389 L390 T391 R392 D393 L394 L395 N396 C397 K400 C401 S402 Y403 V404 V405 T406 L409 G410 V411 N412 V413 F414 K415 D416
P417 V418 A419 D420 P421 N422 K423 R424 S425 K426 K427 G428 R429 L430 S431 L432 H433 T439 F440 V441 T442 L443 E444 E445 G446 K447 G448 D449 L450 E451 E452 L458 V461 F462 K463 K466 V467 S472 F473 D474 E475 V476 R477 Q481 L482 N483 MET GLU GLN ASP VAL ALA PRO HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.89Å 106.08Å 117.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 38.20 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 81.8 (38.20-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.84 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.278 0.229 , 0.277	Depositor DCC
R_{free} test set	1880 reflections (9.86%)	DCC
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Outliers	9 of 20685 reflections (0.044%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7576	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.91 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9071e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NMN

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	0.41	0/3788	0.66	0/5136
1	B	0.39	0/3788	0.65	0/5136
All	All	0.40	0/7576	0.65	0/10272

There are no bond length outliers.

There are no bond angle outliers.

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	3700	0	3665	365	0
1	B	3700	0	3665	344	0
2	A	22	0	14	5	0
2	B	22	0	14	3	0
3	A	82	0	0	7	0
3	B	50	0	0	2	0
All	All	7576	0	7358	666	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 45.

All (666) 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:318:LEU:HD23	1:B:364:ILE:HA	1.22	1.15
1:A:435:THR:HG22	1:A:441:VAL:HG23	1.24	1.09
1:B:400:LYS:HE2	1:B:401:CYS:H	1.08	1.08
1:A:318:LEU:HD23	1:A:364:ILE:HA	1.35	1.06
1:B:365:VAL:HG22	1:B:375:ILE:HD12	1.38	1.04
1:B:386:LEU:HD22	1:B:387:LEU:HD23	1.40	0.99
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.23	0.97
1:A:365:VAL:HG22	1:A:375:ILE:HD12	1.43	0.97
1:A:286:ALA:HA	1:A:290:ILE:HG12	1.47	0.95
1:B:179:THR:HG21	1:B:374:SER:HA	1.47	0.93
1:A:413:VAL:HG21	1:B:252:ALA:HA	1.50	0.91
1:A:11:ILE:HD13	1:A:74:VAL:HB	1.51	0.91
1:A:13:LEU:HA	1:A:87:TYR:OH	1.71	0.91
1:A:97:ASN:HD21	1:A:100:GLY:HA3	1.34	0.90
1:B:400:LYS:HE2	1:B:401:CYS:N	1.87	0.90
1:A:115:GLU:HG3	1:A:463:LYS:HD3	1.54	0.89
1:B:233:THR:HG21	1:B:238:PRO:HB3	1.52	0.89
1:A:433:HIS:CD2	1:A:443:LEU:HD12	2.08	0.89
1:B:112:LEU:HD22	1:B:144:LEU:HD11	1.55	0.88
1:A:253:TRP:O	1:A:257:HIS:HB2	1.75	0.87
1:A:343:LEU:HD11	1:A:349:ARG:HH12	1.42	0.85
1:A:286:ALA:HA	1:A:290:ILE:CG1	2.07	0.84
1:B:415:LYS:H	1:B:425:SER:HB3	1.40	0.82
1:A:272:VAL:HB	1:A:273:PRO:HD2	1.62	0.81
1:A:337:ASN:C	1:A:337:ASN:HD22	1.82	0.81
1:A:13:LEU:HB2	1:B:221:VAL:HG11	1.63	0.81
1:A:40:ARG:HE	1:A:423:LYS:HA	1.45	0.81
1:A:439:THR:HG22	1:A:440:PHE:H	1.46	0.81
1:A:179:THR:HG21	1:A:375:ILE:H	1.45	0.80
1:A:435:THR:HG22	1:A:441:VAL:CG2	2.09	0.80
1:B:182:ASN:HD22	1:B:184:ASP:H	1.27	0.80
1:B:318:LEU:CD2	1:B:364:ILE:HA	2.10	0.80
1:B:97:ASN:HD21	1:B:100:GLY:HA3	1.46	0.80
1:B:202:GLU:HG2	1:B:206:ILE:HD11	1.64	0.79
1:B:450:LEU:O	1:B:452:GLU:HG3	1.83	0.79
1:B:157:TYR:O	1:B:161:VAL:HG23	1.83	0.78
1:A:412:ASN:ND2	1:A:445:GLU:HG2	1.98	0.78
1:A:310:ILE:HD12	1:A:328:LEU:HD11	1.65	0.78
1:A:413:VAL:HG13	1:B:251:THR:HB	1.66	0.77
1:A:337:ASN:HD22	1:A:339:LYS:H	1.32	0.77
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASP:OD1	1:B:236:PRO:HD2	1.84	0.77
1:B:21:THR:HG22	1:B:95:VAL:HG11	1.67	0.77
1:B:120:PRO:HG2	1:B:123:SER:OG	1.85	0.77
1:A:157:TYR:O	1:A:161:VAL:HG23	1.85	0.76
1:A:165:SER:HB3	1:A:214:ASN:HD22	1.51	0.76
1:A:172:LEU:HD13	1:A:189:LYS:HB3	1.68	0.76
1:B:31:SER:O	1:B:139:PRO:HA	1.85	0.75
1:A:9:PHE:O	1:A:79:LYS:HE2	1.86	0.75
1:B:179:THR:CG2	1:B:374:SER:HA	2.17	0.75
1:B:31:SER:HB2	1:B:139:PRO:HB3	1.68	0.75
1:A:198:VAL:HG21	1:A:204:ALA:HB2	1.65	0.75
1:A:251:THR:O	1:B:413:VAL:HG22	1.87	0.75
1:B:337:ASN:HD21	1:B:341:TYR:H	1.33	0.75
1:A:433:HIS:HD2	1:A:443:LEU:HD12	1.52	0.74
1:A:234:LYS:HD2	1:A:234:LYS:N	2.01	0.74
1:A:243:PRO:HB3	1:B:21:THR:HG21	1.69	0.73
1:A:318:LEU:HD21	1:A:367:GLY:HA3	1.72	0.72
1:A:416:ASP:CG	1:A:424:ARG:HG2	2.10	0.72
1:A:252:ALA:HA	1:B:413:VAL:HG21	1.71	0.71
1:B:355:GLY:O	1:B:360:THR:HG21	1.90	0.71
1:B:311:ARG:NH1	2:B:1002:NMN:HN71	1.89	0.71
1:A:19:LYS:HA	1:A:22:HIS:CD2	2.25	0.71
1:B:472:SER:OG	1:B:475:GLU:HG3	1.89	0.71
1:A:120:PRO:HG2	1:A:123:SER:OG	1.91	0.70
1:A:182:ASN:HD22	1:A:184:ASP:H	1.37	0.70
1:A:37:PHE:CZ	1:A:397:CYS:HB3	2.26	0.70
1:A:40:ARG:CB	1:A:40:ARG:HH11	2.05	0.70
1:A:34:TYR:HB3	1:A:403:TYR:HB3	1.73	0.69
1:B:37:PHE:HZ	1:B:397:CYS:HB3	1.54	0.69
1:A:75:VAL:HG23	1:A:110:GLY:O	1.92	0.69
1:B:384:GLY:O	1:B:389:LYS:HB2	1.92	0.69
1:A:343:LEU:HD12	1:A:377:ASN:OD1	1.93	0.69
1:A:187:GLU:OE1	1:A:216:LYS:HD2	1.92	0.68
1:B:114:ILE:HG23	1:B:144:LEU:HD13	1.74	0.68
1:A:264:HIS:O	1:A:268:GLN:HG2	1.93	0.68
1:A:413:VAL:CG2	1:B:252:ALA:HA	2.24	0.68
1:A:201:GLN:HG3	1:B:69:TYR:CE2	2.29	0.68
1:B:415:LYS:HG2	1:B:425:SER:HB2	1.76	0.68
1:A:304:THR:HB	1:A:346:PRO:HB2	1.76	0.68
1:A:351:ILE:HG22	1:A:379:SER:OG	1.94	0.68
1:A:182:ASN:ND2	1:A:184:ASP:H	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LYS:H	1:B:234:LYS:HD2	1.57	0.67
1:A:196:ARG:CG	1:A:196:ARG:HH11	2.02	0.67
1:A:270:SER:HA	1:A:302:ARG:HH12	1.59	0.67
1:A:27:PRO:HG3	1:B:253:TRP:CG	2.30	0.67
1:B:365:VAL:CG2	1:B:375:ILE:HD12	2.19	0.67
1:B:311:ARG:NH1	2:B:1002:NMN:N7	2.41	0.67
1:B:175:TYR:OH	1:B:366:GLU:HG2	1.93	0.67
1:A:196:ARG:NH1	1:A:196:ARG:HG2	2.03	0.67
1:A:472:SER:OG	1:A:475:GLU:HG3	1.95	0.67
1:A:23:TYR:CE2	1:A:24:LYS:HG3	2.30	0.67
1:B:179:THR:HG23	1:B:341:TYR:CG	2.30	0.66
1:A:97:ASN:ND2	1:A:100:GLY:HA3	2.07	0.66
1:B:418:VAL:O	1:B:419:ALA:CB	2.43	0.66
1:A:236:PRO:HB2	1:B:89:GLU:OE1	1.96	0.66
1:B:73:LYS:HE3	1:B:76:THR:HG22	1.77	0.66
1:A:10:ASN:OD1	1:A:12:LEU:N	2.28	0.66
1:B:119:VAL:HG22	1:B:131:LEU:O	1.96	0.66
1:B:337:ASN:ND2	1:B:341:TYR:H	1.93	0.65
1:A:130:VAL:HG12	1:A:442:THR:HG23	1.78	0.65
1:B:386:LEU:HD22	1:B:387:LEU:CD2	2.22	0.65
1:B:365:VAL:HG22	1:B:375:ILE:CD1	2.21	0.65
1:A:435:THR:CG2	1:A:441:VAL:HG23	2.15	0.65
1:B:481:GLN:HE21	1:B:482:LEU:H	1.43	0.65
1:A:36:TYR:CE1	1:A:38:GLU:HG2	2.31	0.65
1:B:326:ASP:OD1	1:B:330:LYS:HE2	1.97	0.65
1:A:462:PHE:CZ	1:A:465:GLY:HA2	2.32	0.65
1:B:273:PRO:HB3	1:B:307:PRO:HD2	1.78	0.65
1:A:234:LYS:H	1:A:234:LYS:HD2	1.63	0.64
1:A:337:ASN:HD21	1:A:339:LYS:HB2	1.63	0.64
1:B:343:LEU:HD11	1:B:349:ARG:NH2	2.12	0.64
1:A:40:ARG:HH21	1:A:423:LYS:HG2	1.63	0.64
1:A:39:CYS:O	1:A:127:ARG:HD2	1.98	0.64
1:B:406:THR:O	1:B:409:LEU:HB3	1.97	0.64
1:A:332:PHE:HB3	1:A:333:PRO:HD2	1.80	0.63
1:A:11:ILE:CD1	1:A:74:VAL:HB	2.27	0.63
1:A:270:SER:HA	1:A:302:ARG:NH1	2.13	0.63
1:B:216:LYS:HG2	1:B:477:ARG:HH22	1.63	0.63
1:B:188:TYR:HE2	1:B:240:TYR:HB3	1.63	0.63
1:A:40:ARG:HB2	1:A:40:ARG:HH11	1.61	0.63
1:B:264:HIS:O	1:B:268:GLN:HG2	1.99	0.63
1:B:88:ARG:HH11	1:B:94:ASP:H	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLU:OE1	1:B:146:ASN:ND2	2.32	0.63
1:B:211:HIS:CD2	1:B:386:LEU:HD11	2.34	0.63
1:A:277:VAL:HG13	1:A:311:ARG:CZ	2.28	0.62
1:A:221:VAL:HG11	1:B:87:TYR:HE2	1.65	0.62
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.34	0.62
1:A:414:PHE:CD2	1:A:427:LYS:HE2	2.34	0.62
1:A:337:ASN:ND2	1:A:339:LYS:H	1.96	0.62
1:A:21:THR:HG22	1:A:95:VAL:HG11	1.80	0.62
1:A:430:LEU:CD2	1:A:444:GLU:HG2	2.30	0.62
1:B:19:LYS:HA	1:B:22:HIS:CG	2.35	0.62
1:A:165:SER:HB3	1:A:214:ASN:ND2	2.13	0.62
1:B:10:ASN:OD1	1:B:12:LEU:HB2	1.98	0.62
1:A:27:PRO:HG3	1:B:253:TRP:CD2	2.35	0.62
1:A:268:GLN:OE1	1:B:24:LYS:HD3	1.99	0.62
1:B:198:VAL:HG21	1:B:204:ALA:HB2	1.82	0.62
1:A:262:PHE:HE2	1:A:286:ALA:HB1	1.63	0.61
1:A:182:ASN:HD22	1:A:183:LEU:N	1.98	0.61
1:A:259:LYS:HG3	1:A:295:LEU:HD21	1.83	0.61
1:A:203:THR:HG23	1:B:199:SER:HB2	1.82	0.61
1:A:263:GLU:HB2	1:A:295:LEU:HD11	1.81	0.61
1:A:388:GLN:HG3	1:A:389:LYS:H	1.65	0.60
1:A:383:GLY:HA3	2:A:1001:NMN:O3P	2.01	0.60
1:B:169:LYS:HG2	1:B:482:LEU:HD11	1.82	0.60
1:A:355:GLY:O	1:A:360:THR:HG21	2.01	0.60
1:B:426:LYS:HD3	1:B:430:LEU:HD13	1.84	0.60
1:B:337:ASN:HD22	1:B:337:ASN:C	2.05	0.60
1:A:56:GLU:HA	1:A:126:PRO:HA	1.82	0.60
1:A:78:GLU:CD	1:A:78:GLU:H	2.04	0.60
1:A:32:LYS:NZ	1:A:32:LYS:HB2	2.16	0.60
1:B:358:ILE:HG23	1:B:359:ASN:H	1.66	0.60
1:A:450:LEU:O	1:A:452:GLU:N	2.35	0.60
1:A:246:GLU:HG3	1:A:248:SER:H	1.66	0.59
1:A:175:TYR:CE2	1:A:366:GLU:HG2	2.37	0.59
1:A:262:PHE:CE2	1:A:286:ALA:HB1	2.37	0.59
1:A:13:LEU:HA	1:A:87:TYR:HH	1.68	0.59
1:B:13:LEU:HD21	1:B:83:ALA:HA	1.84	0.59
1:A:55:GLU:O	1:A:126:PRO:HA	2.02	0.59
1:A:240:TYR:HA	1:B:90:HIS:CD2	2.38	0.59
1:B:473:PHE:O	1:B:477:ARG:HG3	2.03	0.59
1:B:323:LYS:O	1:B:327:ILE:HG13	2.02	0.59
1:B:30:THR:HG23	1:B:404:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:O	1:A:389:LYS:HB3	2.03	0.59
1:B:76:THR:O	1:B:80:ILE:HG13	2.03	0.59
1:B:388:GLN:HG3	1:B:389:LYS:N	2.18	0.58
1:A:119:VAL:HG22	1:A:131:LEU:O	2.03	0.58
1:A:170:LYS:HG2	1:A:482:LEU:HD22	1.86	0.58
1:B:56:GLU:HA	1:B:126:PRO:HA	1.85	0.58
1:A:33:VAL:HG13	1:A:145:THR:CB	2.33	0.58
1:B:39:CYS:O	1:B:127:ARG:HG3	2.03	0.58
1:A:310:ILE:HD12	1:A:328:LEU:CD1	2.33	0.58
1:B:234:LYS:HD2	1:B:234:LYS:N	2.18	0.58
1:B:57:THR:CG2	1:B:395:LEU:HD13	2.34	0.58
1:A:28:PRO:O	1:A:29:ASN:HB2	2.04	0.58
1:A:115:GLU:HG3	1:A:463:LYS:CD	2.28	0.58
1:B:194:GLY:O	1:B:198:VAL:HG13	2.03	0.58
1:A:432:LEU:CD1	1:A:457:LEU:HD12	2.34	0.58
1:B:231:TYR:O	1:B:472:SER:HA	2.03	0.58
1:A:195:TYR:OH	1:B:14:ALA:HA	2.04	0.58
1:A:175:TYR:O	1:A:179:THR:HB	2.02	0.58
1:A:237:VAL:HG23	1:B:89:GLU:HG2	1.86	0.58
1:B:75:VAL:HB	1:B:110:GLY:HA2	1.86	0.58
1:A:19:LYS:HG2	1:A:22:HIS:CD2	2.39	0.57
1:A:384:GLY:O	1:A:388:GLN:O	2.22	0.57
1:B:342:LYS:HD3	1:B:372:LYS:O	2.04	0.57
1:B:113:PRO:HG3	1:B:141:CYS:SG	2.44	0.57
1:A:413:VAL:HG13	1:B:251:THR:CB	2.35	0.57
1:B:9:PHE:CZ	1:B:69:TYR:HD2	2.22	0.57
1:B:195:TYR:CG	1:B:220:THR:HG23	2.39	0.57
1:B:19:LYS:HG2	1:B:22:HIS:CD2	2.40	0.57
1:A:282:ASP:H	1:B:418:VAL:HG23	1.70	0.57
1:A:129:ASN:HA	1:A:442:THR:OG1	2.04	0.57
1:A:116:VAL:CG2	1:A:462:PHE:HB3	2.34	0.57
1:A:450:LEU:C	1:A:452:GLU:H	2.07	0.56
1:B:278:SER:HB2	1:B:286:ALA:HB3	1.87	0.56
1:A:337:ASN:C	1:A:337:ASN:ND2	2.56	0.56
1:A:10:ASN:OD1	1:A:12:LEU:HB2	2.05	0.56
1:A:311:ARG:CZ	2:A:1001:NMN:HN71	2.18	0.56
1:B:284:TYR:CZ	1:B:323:LYS:HD3	2.41	0.56
1:A:175:TYR:CG	1:A:365:VAL:HG13	2.41	0.56
3:A:1006:HOH:O	1:B:389:LYS:N	2.36	0.56
1:A:386:LEU:HD12	1:A:386:LEU:O	2.05	0.56
1:B:433:HIS:HB2	1:B:441:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:CD2	1:A:365:VAL:HG13	2.39	0.56
1:A:17:SER:O	1:A:91:PHE:HZ	1.89	0.56
1:B:358:ILE:HG23	1:B:359:ASN:N	2.21	0.56
1:B:187:GLU:OE1	1:B:216:LYS:HD2	2.06	0.56
1:B:116:VAL:HG22	1:B:134:VAL:HG22	1.87	0.56
1:B:71:LYS:HB3	1:B:462:PHE:HE1	1.71	0.56
1:B:23:TYR:CD1	1:B:24:LYS:N	2.74	0.56
1:A:434:ARG:HB2	1:A:434:ARG:CZ	2.34	0.56
1:B:95:VAL:O	1:B:95:VAL:HG12	2.06	0.56
1:A:273:PRO:HB3	1:A:307:PRO:HD2	1.88	0.55
1:B:388:GLN:HG3	1:B:389:LYS:H	1.69	0.55
1:B:311:ARG:CZ	2:B:1002:NMN:HN71	2.19	0.55
1:B:63:GLN:HB3	1:B:231:TYR:CZ	2.41	0.55
1:B:421:PRO:C	1:B:423:LYS:H	2.08	0.55
1:B:40:ARG:HH11	1:B:40:ARG:HG3	1.71	0.55
1:B:412:ASN:ND2	1:B:445:GLU:HG2	2.21	0.55
1:B:175:TYR:CG	1:B:365:VAL:HG13	2.40	0.55
1:B:161:VAL:HG22	1:B:390:LEU:HD12	1.87	0.55
1:B:481:GLN:NE2	1:B:482:LEU:H	2.04	0.55
1:A:88:ARG:HH11	1:A:94:ASP:N	2.05	0.55
1:B:82:GLU:O	1:B:86:VAL:HG23	2.06	0.55
1:A:175:TYR:OH	1:A:366:GLU:HG2	2.07	0.55
1:A:366:GLU:O	1:A:370:GLN:HG3	2.07	0.55
1:A:304:THR:HG22	3:A:1055:HOH:O	2.07	0.55
1:B:177:LEU:HB2	1:B:183:LEU:HD21	1.89	0.55
1:A:186:LEU:O	1:A:186:LEU:HD22	2.07	0.55
1:B:130:VAL:O	1:B:130:VAL:HG13	2.06	0.55
1:A:33:VAL:HG13	1:A:145:THR:HB	1.89	0.54
1:A:357:ASP:OD2	1:A:357:ASP:C	2.46	0.54
1:A:412:ASN:HD22	1:A:445:GLU:HG2	1.71	0.54
1:A:298:LEU:O	1:A:302:ARG:HG3	2.07	0.54
1:A:40:ARG:NH1	1:A:40:ARG:HB3	2.22	0.54
1:B:392:ARG:CB	1:B:392:ARG:HH11	2.21	0.54
1:A:112:LEU:HD22	1:A:144:LEU:HD11	1.89	0.54
1:B:325:LEU:HD11	1:B:368:MET:HE3	1.90	0.54
1:B:54:TYR:HB2	3:B:1049:HOH:O	2.08	0.54
1:A:11:ILE:HD12	1:A:11:ILE:H	1.72	0.54
1:A:432:LEU:HD12	1:A:457:LEU:HB2	1.90	0.54
1:B:413:VAL:O	1:B:414:PHE:HB3	2.08	0.54
1:A:390:LEU:HD12	1:A:394:LEU:HD22	1.90	0.54
1:A:116:VAL:HG23	1:A:462:PHE:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HG23	1:A:238:PRO:HD2	1.90	0.54
1:B:445:GLU:OE1	1:B:447:LYS:HE3	2.08	0.54
1:A:418:VAL:CG1	1:B:282:ASP:HA	2.37	0.54
1:A:40:ARG:CB	1:A:40:ARG:NH1	2.69	0.53
1:B:16:ASP:CB	1:B:18:TYR:HE2	2.21	0.53
1:A:69:TYR:CE2	1:B:201:GLN:HG3	2.42	0.53
1:A:153:VAL:HG22	1:A:399:PHE:HB2	1.90	0.53
1:B:165:SER:HB3	1:B:214:ASN:HD22	1.73	0.53
1:A:194:GLY:O	1:A:198:VAL:HG13	2.07	0.53
1:A:382:SER:N	3:A:1057:HOH:O	2.41	0.53
1:A:105:LEU:O	1:A:105:LEU:HD12	2.09	0.53
1:B:318:LEU:HD21	1:B:367:GLY:HA3	1.90	0.53
1:B:36:TYR:HB2	1:B:130:VAL:HG23	1.91	0.53
1:B:449:ASP:C	1:B:451:GLU:H	2.12	0.53
1:B:304:THR:HB	1:B:346:PRO:HB2	1.91	0.53
1:A:31:SER:O	1:A:139:PRO:HA	2.09	0.53
1:B:67:ASN:ND2	1:B:467:VAL:HG21	2.24	0.53
1:A:368:MET:CE	1:A:380:PHE:HZ	2.22	0.53
1:B:151:ILE:CG2	1:B:152:LEU:N	2.71	0.53
1:A:345:PRO:O	1:A:347:TYR:N	2.42	0.53
1:A:54:TYR:OH	1:A:164:ASN:ND2	2.41	0.53
1:A:175:TYR:OH	1:A:366:GLU:CG	2.57	0.53
1:B:405:VAL:HG22	1:B:410:GLY:HA2	1.91	0.53
1:B:31:SER:HB2	1:B:139:PRO:CB	2.38	0.53
1:A:212:LEU:HD21	1:A:218:THR:HB	1.91	0.53
1:A:69:TYR:CB	1:A:151:ILE:HD11	2.39	0.52
1:B:119:VAL:HG13	1:B:458:LEU:HD23	1.91	0.52
1:B:278:SER:HB2	1:B:286:ALA:CB	2.38	0.52
1:A:263:GLU:HB2	1:A:295:LEU:CD1	2.39	0.52
1:A:156:TRP:HH2	1:B:388:GLN:HE21	1.55	0.52
1:A:211:HIS:CE1	1:A:215:PHE:HB2	2.44	0.52
1:B:392:ARG:HG3	1:B:397:CYS:HB2	1.92	0.52
1:A:391:THR:HG21	1:B:389:LYS:HG2	1.90	0.52
1:B:9:PHE:CG	1:B:10:ASN:N	2.78	0.52
1:A:62:LEU:O	1:A:66:LEU:HG	2.09	0.52
1:A:227:ILE:HD13	1:A:473:PHE:CE2	2.44	0.52
1:A:329:GLY:HA2	1:A:334:VAL:HG13	1.92	0.52
1:A:33:VAL:HG11	1:A:142:TYR:O	2.10	0.52
1:A:357:ASP:H	1:A:360:THR:HB	1.74	0.52
1:A:78:GLU:CD	1:A:78:GLU:N	2.64	0.52
1:B:81:GLN:O	1:B:85:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLN:O	1:B:366:GLU:HB2	2.10	0.52
1:B:351:ILE:HG23	1:B:351:ILE:O	2.10	0.52
1:A:113:PRO:HG3	1:A:141:CYS:SG	2.49	0.52
1:A:19:LYS:NZ	1:B:246:GLU:OE1	2.35	0.52
1:B:426:LYS:HE2	1:B:442:THR:HG21	1.90	0.52
1:A:450:LEU:HB2	1:A:452:GLU:HG2	1.91	0.52
1:A:179:THR:CG2	1:A:374:SER:HA	2.40	0.51
1:B:392:ARG:HB3	1:B:392:ARG:NH1	2.25	0.51
1:A:224:ILE:HG12	1:A:238:PRO:HG2	1.93	0.51
1:B:202:GLU:HG2	1:B:206:ILE:CD1	2.39	0.51
1:B:156:TRP:HH2	1:B:390:LEU:O	1.92	0.51
1:B:59:PHE:CD2	1:B:119:VAL:HG23	2.46	0.51
1:A:40:ARG:O	1:A:127:ARG:NH1	2.43	0.51
1:A:68:LYS:HD3	1:A:69:TYR:CE1	2.46	0.51
1:A:36:TYR:HE1	1:A:38:GLU:HG2	1.73	0.51
1:B:104:ILE:HD12	1:B:104:ILE:N	2.25	0.51
1:B:392:ARG:HB3	1:B:392:ARG:HH11	1.76	0.51
1:A:37:PHE:HZ	1:A:397:CYS:HB3	1.72	0.51
1:B:449:ASP:O	1:B:451:GLU:N	2.35	0.51
1:B:21:THR:HG22	1:B:95:VAL:CG1	2.39	0.51
1:B:175:TYR:CD2	1:B:365:VAL:HG13	2.46	0.51
1:A:439:THR:HG22	1:A:440:PHE:N	2.21	0.51
1:A:212:LEU:HA	1:A:215:PHE:O	2.11	0.51
1:A:88:ARG:NH1	1:A:94:ASP:H	2.09	0.51
1:A:12:LEU:O	1:A:147:TRP:HZ2	1.94	0.51
1:B:68:LYS:HD3	1:B:69:TYR:CE1	2.46	0.51
1:A:27:PRO:HG3	1:B:253:TRP:CD1	2.46	0.50
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.93	0.50
1:A:290:ILE:HG22	1:A:295:LEU:HD23	1.93	0.50
1:A:130:VAL:CG1	1:A:442:THR:HG23	2.42	0.50
1:B:151:ILE:HG23	1:B:152:LEU:N	2.26	0.50
1:B:36:TYR:HE1	1:B:38:GLU:HG2	1.77	0.50
1:B:9:PHE:O	1:B:79:LYS:HE2	2.12	0.50
1:A:259:LYS:HG3	1:A:295:LEU:CD2	2.41	0.50
1:A:33:VAL:HG13	1:A:33:VAL:O	2.12	0.50
1:B:57:THR:HG22	1:B:395:LEU:HD13	1.92	0.50
1:A:236:PRO:HB2	1:B:89:GLU:CD	2.31	0.50
1:B:294:ASP:O	1:B:295:LEU:HD23	2.12	0.50
1:A:324:VAL:O	1:A:328:LEU:HG	2.12	0.50
1:B:134:VAL:HG21	1:B:152:LEU:CD1	2.41	0.50
1:A:325:LEU:HB3	1:A:373:TRP:CZ2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:SER:C	1:B:376:GLU:H	2.15	0.50
1:A:119:VAL:HG13	1:A:458:LEU:HD23	1.93	0.50
1:A:244:ALA:CB	1:A:275:SER:HB3	2.42	0.50
1:A:247:HIS:HE1	1:A:279:ASP:OD2	1.95	0.50
1:A:278:SER:O	1:A:283:ILE:HA	2.12	0.50
1:A:246:GLU:OE2	1:B:19:LYS:NZ	2.35	0.49
1:B:443:LEU:HD12	1:B:448:GLY:HA2	1.94	0.49
1:B:103:TYR:HE2	1:B:138:ASP:OD1	1.94	0.49
1:A:263:GLU:HA	1:A:266:VAL:HG22	1.93	0.49
1:A:312:PRO:HD2	1:A:351:ILE:O	2.12	0.49
1:A:357:ASP:OD2	1:A:359:ASN:N	2.45	0.49
1:A:58:VAL:CG2	1:A:166:ARG:HD3	2.42	0.49
1:A:252:ALA:HA	1:B:413:VAL:CG2	2.40	0.49
1:B:11:ILE:HG23	1:B:12:LEU:HD23	1.93	0.49
1:B:28:PRO:O	1:B:29:ASN:HB2	2.12	0.49
1:B:357:ASP:OD2	1:B:357:ASP:C	2.50	0.49
1:B:378:VAL:HG12	1:B:379:SER:N	2.27	0.49
1:A:272:VAL:HB	1:A:273:PRO:CD	2.39	0.49
1:A:15:THR:OG1	1:A:19:LYS:HD2	2.13	0.49
1:A:164:ASN:O	1:A:168:GLN:HG3	2.12	0.49
1:B:103:TYR:CZ	1:B:107:LYS:HG3	2.47	0.49
1:B:34:TYR:CE2	1:B:429:ARG:HA	2.47	0.49
1:B:391:THR:H	1:B:394:LEU:HD13	1.76	0.49
1:B:318:LEU:C	1:B:318:LEU:HD13	2.32	0.49
1:A:388:GLN:HG3	1:A:389:LYS:N	2.27	0.49
1:A:300:VAL:HG22	1:A:347:TYR:OH	2.13	0.49
1:A:10:ASN:OD1	1:A:10:ASN:C	2.50	0.49
1:A:418:VAL:HG13	1:A:419:ALA:N	2.28	0.49
1:B:63:GLN:HB3	1:B:231:TYR:OH	2.12	0.48
1:B:80:ILE:CD1	1:B:105:LEU:HD22	2.43	0.48
1:B:432:LEU:HB2	1:B:458:LEU:HG	1.93	0.48
1:A:278:SER:HB2	1:A:283:ILE:CD1	2.43	0.48
1:B:68:LYS:HD3	1:B:69:TYR:HE1	1.78	0.48
1:A:295:LEU:HD12	1:A:298:LEU:HD12	1.95	0.48
1:B:104:ILE:HD11	1:B:141:CYS:SG	2.53	0.48
1:A:337:ASN:ND2	1:A:339:LYS:N	2.60	0.48
1:A:128:GLY:O	1:A:426:LYS:HE2	2.13	0.48
1:B:88:ARG:HH11	1:B:94:ASP:N	2.12	0.48
1:B:148:ILE:O	1:B:151:ILE:HG22	2.12	0.48
1:A:114:ILE:CG2	1:A:144:LEU:HD13	2.43	0.48
1:A:375:ILE:HG22	1:A:375:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PHE:CZ	1:A:69:TYR:HD2	2.31	0.48
1:B:288:GLU:O	1:B:292:GLY:HA3	2.13	0.48
1:B:320:THR:O	1:B:324:VAL:HG23	2.14	0.48
1:B:418:VAL:O	1:B:419:ALA:HB2	2.12	0.48
1:B:169:LYS:HB2	1:B:215:PHE:CZ	2.48	0.48
1:B:237:VAL:HG11	1:B:240:TYR:HB2	1.95	0.48
1:A:202:GLU:HG2	1:B:200:SER:HB2	1.95	0.48
1:B:67:ASN:N	1:B:67:ASN:HD22	2.12	0.48
1:A:25:GLN:HG2	1:B:265:ILE:HG12	1.95	0.47
1:B:21:THR:C	1:B:25:GLN:HE21	2.17	0.47
1:B:80:ILE:HD11	1:B:105:LEU:HD22	1.96	0.47
1:B:13:LEU:HA	1:B:87:TYR:OH	2.15	0.47
1:B:423:LYS:O	1:B:423:LYS:HG2	2.13	0.47
1:A:196:ARG:HB3	1:B:150:THR:HG23	1.96	0.47
1:B:433:HIS:HD2	1:B:443:LEU:HG	1.78	0.47
1:B:394:LEU:C	1:B:396:ASN:H	2.17	0.47
1:B:104:ILE:H	1:B:104:ILE:HD12	1.79	0.47
1:A:432:LEU:HD12	1:A:457:LEU:HD12	1.96	0.47
1:B:384:GLY:O	1:B:388:GLN:O	2.32	0.47
1:B:309:ILE:HG22	1:B:351:ILE:HG22	1.95	0.47
1:A:219:ASP:CG	1:B:17:SER:HB2	2.35	0.47
1:A:76:THR:O	1:A:80:ILE:HG13	2.14	0.47
1:B:345:PRO:HB2	1:B:347:TYR:CE2	2.49	0.47
1:B:155:SER:O	1:B:158:PRO:HG2	2.15	0.47
1:B:275:SER:HA	1:B:309:ILE:HB	1.96	0.47
1:B:17:SER:OG	1:B:90:HIS:HE1	1.96	0.47
1:B:283:ILE:HG23	1:B:284:TYR:N	2.28	0.47
1:B:134:VAL:HG21	1:B:152:LEU:HD13	1.96	0.47
1:B:172:LEU:HD13	1:B:189:LYS:HB2	1.96	0.47
1:A:205:GLY:O	1:A:223:GLY:HA2	2.15	0.47
1:A:114:ILE:HG23	1:A:144:LEU:HD13	1.97	0.47
1:A:235:ASP:HB3	3:A:1011:HOH:O	2.15	0.47
1:A:175:TYR:HE2	1:A:366:GLU:HG2	1.79	0.47
1:B:157:TYR:HB3	1:B:158:PRO:CD	2.44	0.47
1:A:174:LYS:O	1:A:178:GLU:HG2	2.14	0.47
1:A:281:TYR:O	1:A:282:ASP:C	2.53	0.46
1:B:136:ASN:CG	1:B:142:TYR:HA	2.36	0.46
1:A:243:PRO:CB	1:B:21:THR:HG21	2.41	0.46
1:A:182:ASN:ND2	1:A:182:ASN:C	2.69	0.46
1:A:205:GLY:CA	1:A:222:ALA:HB1	2.46	0.46
1:A:265:ILE:O	1:A:269:PHE:HD1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HG3	1:A:72:GLY:N	2.30	0.46
1:A:84:LYS:HD3	1:A:98:GLU:OE1	2.15	0.46
1:A:365:VAL:HG22	1:A:375:ILE:CD1	2.31	0.46
1:A:337:ASN:ND2	1:A:339:LYS:HB2	2.30	0.46
1:A:68:LYS:HG2	1:A:69:TYR:CE1	2.51	0.46
1:A:36:TYR:CE1	1:A:426:LYS:HD2	2.50	0.46
1:B:17:SER:O	1:B:20:VAL:HG23	2.14	0.46
1:B:55:GLU:O	1:B:127:ARG:HB2	2.15	0.46
1:A:205:GLY:HA2	1:A:222:ALA:HB1	1.97	0.46
1:B:116:VAL:HG13	1:B:133:THR:O	2.16	0.46
1:B:165:SER:OG	1:B:211:HIS:CD2	2.68	0.46
1:A:13:LEU:CB	1:B:221:VAL:HG11	2.40	0.46
1:B:114:ILE:CG2	1:B:144:LEU:HD13	2.42	0.46
1:B:430:LEU:HD22	1:B:444:GLU:HG2	1.97	0.46
1:A:212:LEU:O	1:A:477:ARG:NH2	2.49	0.46
1:B:292:GLY:C	1:B:296:ARG:HG2	2.35	0.46
1:A:33:VAL:CG1	1:A:142:TYR:O	2.64	0.46
1:B:433:HIS:CD2	1:B:443:LEU:HG	2.51	0.46
1:A:67:ASN:HA	1:A:71:LYS:HE2	1.98	0.46
1:A:178:GLU:HB2	3:A:1018:HOH:O	2.16	0.46
1:A:32:LYS:HA	1:A:136:ASN:OD1	2.16	0.46
1:B:127:ARG:HG2	1:B:127:ARG:NH1	2.30	0.46
1:A:467:VAL:HG12	3:A:1064:HOH:O	2.16	0.46
1:B:109:ASP:O	1:B:111:HIS:HD2	1.99	0.46
1:B:161:VAL:HG22	1:B:390:LEU:CD1	2.46	0.46
1:B:36:TYR:HA	1:B:133:THR:HA	1.98	0.46
1:A:34:TYR:CB	1:A:403:TYR:HB3	2.43	0.45
1:A:350:VAL:CG1	1:A:351:ILE:N	2.79	0.45
1:B:343:LEU:HD12	1:B:344:LEU:N	2.30	0.45
1:B:483:ASN:HB3	3:B:1034:HOH:O	2.16	0.45
1:B:39:CYS:HB3	1:B:127:ARG:HD2	1.98	0.45
1:B:233:THR:O	1:B:233:THR:HG23	2.16	0.45
1:A:176:LEU:HD22	1:A:182:ASN:O	2.17	0.45
1:B:54:TYR:OH	1:B:164:ASN:ND2	2.49	0.45
1:B:305:GLU:HG2	1:B:305:GLU:O	2.15	0.45
1:A:314:SER:HB3	1:B:419:ALA:HB3	1.99	0.45
1:B:59:PHE:O	1:B:121:GLU:HA	2.17	0.45
1:A:145:THR:HG22	1:A:146:ASN:HD22	1.80	0.45
1:A:420:ASP:OD1	1:A:423:LYS:HG3	2.16	0.45
1:A:332:PHE:CD2	1:A:348:LEU:HD22	2.52	0.45
1:B:146:ASN:O	1:B:147:TRP:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HB2	1:B:221:VAL:CG1	2.41	0.45
1:A:120:PRO:HG2	1:A:123:SER:HG	1.81	0.45
1:A:277:VAL:HA	1:A:311:ARG:O	2.17	0.45
1:B:88:ARG:HD3	1:B:94:ASP:CG	2.36	0.45
1:B:310:ILE:HD12	1:B:328:LEU:HD11	1.98	0.45
1:B:18:TYR:CE2	1:B:19:LYS:HG3	2.52	0.45
1:B:413:VAL:CG1	1:B:414:PHE:N	2.79	0.45
1:A:73:LYS:HE3	1:A:76:THR:HG22	1.99	0.45
1:B:37:PHE:HB2	1:B:132:PHE:CZ	2.52	0.44
1:A:36:TYR:CZ	1:A:426:LYS:HB2	2.53	0.44
1:A:196:ARG:NH2	1:B:16:ASP:OD2	2.50	0.44
1:A:17:SER:OG	1:B:219:ASP:HA	2.17	0.44
1:B:386:LEU:C	1:B:386:LEU:CD2	2.85	0.44
1:A:175:TYR:CZ	1:A:366:GLU:HG2	2.52	0.44
1:A:272:VAL:C	1:A:306:ALA:HB1	2.37	0.44
1:B:304:THR:O	1:B:307:PRO:HD3	2.18	0.44
1:A:289:LYS:HE3	1:A:289:LYS:HB2	1.83	0.44
1:B:366:GLU:O	1:B:370:GLN:HG3	2.17	0.44
1:B:16:ASP:CB	1:B:18:TYR:CE2	3.00	0.44
1:A:365:VAL:CG2	1:A:375:ILE:HD12	2.31	0.44
1:B:202:GLU:O	1:B:206:ILE:HG13	2.17	0.44
1:B:262:PHE:CE2	1:B:286:ALA:HB1	2.52	0.44
1:A:434:ARG:HG3	1:A:434:ARG:HH11	1.83	0.44
1:A:149:GLU:HG2	1:A:150:THR:N	2.33	0.44
1:B:391:THR:C	1:B:393:ASP:N	2.71	0.44
1:B:242:VAL:HB	1:B:243:PRO:HD2	1.99	0.44
1:A:169:LYS:HD2	1:A:214:ASN:O	2.17	0.44
1:B:183:LEU:O	1:B:186:LEU:HB2	2.17	0.44
1:B:309:ILE:N	1:B:309:ILE:HD12	2.32	0.44
1:A:146:ASN:N	1:A:146:ASN:HD22	2.14	0.44
1:A:33:VAL:HG23	1:A:401:CYS:SG	2.58	0.44
1:A:33:VAL:O	1:A:145:THR:HG21	2.18	0.44
1:A:231:TYR:O	1:A:472:SER:HA	2.18	0.44
1:B:421:PRO:C	1:B:423:LYS:N	2.71	0.44
1:B:168:GLN:OE1	1:B:190:LEU:HD11	2.18	0.44
1:A:169:LYS:HG2	1:A:482:LEU:HD11	1.99	0.44
1:A:12:LEU:HD21	1:A:75:VAL:HG13	1.99	0.44
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.82	0.44
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.67	0.43
1:B:55:GLU:O	1:B:127:ARG:N	2.42	0.43
1:B:36:TYR:CE1	1:B:38:GLU:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:O	1:A:153:VAL:HG23	2.17	0.43
1:B:16:ASP:HB2	1:B:18:TYR:HE2	1.83	0.43
1:B:33:VAL:CG1	1:B:145:THR:HB	2.48	0.43
1:B:172:LEU:HD13	1:B:189:LYS:CB	2.48	0.43
1:B:84:LYS:HA	1:B:96:PHE:CD2	2.53	0.43
1:A:262:PHE:HB3	1:A:291:TRP:CH2	2.53	0.43
1:B:262:PHE:HE2	1:B:286:ALA:HB1	1.83	0.43
1:A:300:VAL:HA	1:A:347:TYR:CE2	2.54	0.43
1:A:384:GLY:N	2:A:1001:NMN:O3P	2.49	0.43
1:B:253:TRP:O	1:B:257:HIS:HB2	2.18	0.43
1:A:114:ILE:HG13	1:A:114:ILE:O	2.18	0.43
1:B:374:SER:C	1:B:376:GLU:N	2.72	0.43
1:B:216:LYS:HG2	1:B:477:ARG:NH2	2.31	0.43
1:B:34:TYR:HD1	1:B:135:GLU:HB3	1.83	0.43
1:A:157:TYR:HB3	1:A:158:PRO:CD	2.49	0.43
1:A:391:THR:HB	1:A:393:ASP:OD2	2.19	0.43
1:B:304:THR:CG2	1:B:346:PRO:HB2	2.48	0.43
1:A:284:TYR:HE2	1:A:323:LYS:HB3	1.83	0.43
1:B:33:VAL:HG12	1:B:145:THR:HB	2.01	0.43
1:B:19:LYS:HG2	1:B:22:HIS:NE2	2.33	0.43
1:A:311:ARG:NH1	2:A:1001:NMN:HN71	2.17	0.43
1:B:141:CYS:HB3	1:B:144:LEU:HB2	2.01	0.43
1:B:115:GLU:HA	1:B:462:PHE:O	2.19	0.43
1:B:403:TYR:CD2	1:B:429:ARG:HG2	2.54	0.43
1:B:293:GLU:OE1	1:B:331:LYS:NZ	2.47	0.43
1:B:415:LYS:N	1:B:425:SER:HB3	2.21	0.43
1:B:312:PRO:HD2	1:B:351:ILE:O	2.19	0.43
1:B:441:VAL:O	1:B:441:VAL:HG13	2.18	0.43
1:B:91:PHE:CD1	1:B:91:PHE:N	2.86	0.43
1:A:244:ALA:HB2	1:A:275:SER:HB3	2.00	0.42
1:A:263:GLU:HG3	1:A:298:LEU:HD11	2.01	0.42
1:B:449:ASP:C	1:B:451:GLU:N	2.73	0.42
1:A:10:ASN:CG	1:A:79:LYS:HD2	2.39	0.42
1:A:198:VAL:HG12	1:A:387:LEU:HB3	2.01	0.42
1:A:142:TYR:CD2	1:A:142:TYR:N	2.86	0.42
1:B:431:SER:HB2	1:B:433:HIS:NE2	2.34	0.42
1:B:153:VAL:C	1:B:155:SER:N	2.73	0.42
1:B:388:GLN:O	1:B:389:LYS:CB	2.66	0.42
1:A:20:VAL:HA	1:A:147:TRP:CZ3	2.54	0.42
1:A:311:ARG:NH1	2:A:1001:NMN:N7	2.67	0.42
1:B:34:TYR:CD2	1:B:403:TYR:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HB	1:B:142:TYR:O	2.19	0.42
1:B:279:ASP:O	1:B:280:SER:C	2.57	0.42
1:A:101:TRP:CE2	1:A:143:TRP:HH2	2.37	0.42
1:B:35:SER:OG	1:B:401:CYS:HA	2.19	0.42
1:A:115:GLU:HA	1:A:462:PHE:O	2.20	0.42
1:B:277:VAL:HG13	1:B:311:ARG:CZ	2.49	0.42
1:A:182:ASN:HD22	1:A:182:ASN:C	2.21	0.42
1:A:117:LYS:HB2	1:A:133:THR:OG1	2.19	0.42
1:B:17:SER:OG	1:B:90:HIS:CE1	2.72	0.42
1:A:191:HIS:ND1	1:A:193:PHE:HE1	2.18	0.42
1:A:390:LEU:HD12	1:A:394:LEU:CD2	2.49	0.42
1:A:344:LEU:HB3	1:A:345:PRO:HD2	2.00	0.42
1:A:317:PRO:HB2	1:A:364:ILE:HD11	2.02	0.42
1:A:374:SER:C	1:A:376:GLU:H	2.23	0.42
1:A:33:VAL:CG1	1:A:145:THR:HB	2.49	0.42
1:B:102:ASN:O	1:B:105:LEU:HB3	2.19	0.42
1:B:283:ILE:HG23	1:B:284:TYR:CD2	2.55	0.42
1:B:412:ASN:HB3	1:B:427:LYS:HB2	2.00	0.42
1:A:422:ASN:HA	1:A:422:ASN:HD22	1.57	0.42
1:B:350:VAL:HG12	1:B:351:ILE:N	2.35	0.42
1:B:119:VAL:CG1	1:B:432:LEU:HD12	2.49	0.42
1:A:195:TYR:CG	1:A:220:THR:HG23	2.55	0.42
1:B:415:LYS:H	1:B:425:SER:CB	2.20	0.42
1:A:145:THR:HG22	1:A:146:ASN:ND2	2.35	0.42
1:B:115:GLU:HG3	1:B:463:LYS:HG2	2.00	0.42
1:A:81:GLN:O	1:A:85:GLU:HG3	2.20	0.42
1:A:404:VAL:O	1:A:411:VAL:HG22	2.19	0.42
1:B:402:SER:O	1:B:428:GLY:N	2.51	0.42
1:A:179:THR:HG23	1:A:374:SER:HA	2.02	0.42
1:A:116:VAL:HB	1:A:462:PHE:HB3	2.00	0.42
1:B:153:VAL:C	1:B:155:SER:H	2.23	0.42
1:A:9:PHE:CG	1:A:10:ASN:N	2.88	0.42
1:B:405:VAL:HA	1:B:409:LEU:O	2.19	0.42
1:B:325:LEU:HB3	1:B:373:TRP:CZ2	2.55	0.42
1:A:432:LEU:HD11	1:A:440:PHE:HD2	1.85	0.42
1:A:37:PHE:HA	1:A:398:SER:O	2.20	0.42
1:B:11:ILE:HG23	1:B:12:LEU:CD2	2.50	0.42
1:B:121:GLU:HB2	1:B:476:VAL:HG22	2.00	0.42
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.87	0.42
1:B:111:HIS:CE1	1:B:466:LYS:HE3	2.55	0.42
1:A:173:ALA:HA	1:A:183:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:VAL:CG1	1:B:379:SER:N	2.83	0.42
1:B:178:GLU:HG2	1:B:178:GLU:O	2.19	0.42
1:B:179:THR:HG23	1:B:341:TYR:CD2	2.55	0.41
1:B:449:ASP:O	1:B:451:GLU:HG3	2.20	0.41
1:B:198:VAL:HA	1:B:388:GLN:HB2	2.02	0.41
1:A:128:GLY:O	1:A:426:LYS:CE	2.68	0.41
1:B:284:TYR:CE2	1:B:323:LYS:HB3	2.55	0.41
1:A:35:SER:HB3	1:A:399:PHE:CE2	2.55	0.41
1:B:391:THR:OG1	1:B:393:ASP:HB2	2.20	0.41
1:A:337:ASN:HD22	1:A:339:LYS:N	2.07	0.41
1:B:123:SER:HB3	1:B:125:ILE:HD11	2.00	0.41
1:A:156:TRP:CD2	1:A:157:TYR:N	2.88	0.41
1:A:482:LEU:HB3	1:A:483:ASN:H	1.75	0.41
1:A:388:GLN:O	1:A:389:LYS:CB	2.64	0.41
1:B:116:VAL:O	1:B:461:VAL:HG22	2.20	0.41
1:B:40:ARG:NE	1:B:423:LYS:HA	2.35	0.41
1:A:134:VAL:HG21	1:A:152:LEU:HD13	2.02	0.41
1:B:386:LEU:C	1:B:386:LEU:HD23	2.40	0.41
1:A:23:TYR:CZ	1:A:24:LYS:HG3	2.55	0.41
1:A:32:LYS:HZ2	1:A:32:LYS:HB2	1.84	0.41
1:A:191:HIS:HA	1:A:217:GLY:O	2.20	0.41
1:B:191:HIS:CE1	1:B:219:ASP:OD1	2.73	0.41
1:B:299:ILE:HG22	1:B:347:TYR:CD1	2.55	0.41
1:A:317:PRO:O	1:A:321:VAL:HG23	2.21	0.41
1:A:368:MET:HE2	1:A:380:PHE:HZ	1.85	0.41
1:B:114:ILE:O	1:B:114:ILE:HG13	2.20	0.41
1:A:253:TRP:CG	1:B:27:PRO:HG3	2.56	0.41
1:A:423:LYS:O	1:A:424:ARG:C	2.59	0.41
1:A:350:VAL:HG12	1:A:351:ILE:N	2.35	0.41
1:B:450:LEU:O	1:B:451:GLU:C	2.59	0.41
1:B:156:TRP:CG	1:B:157:TYR:N	2.89	0.41
1:A:130:VAL:O	1:A:130:VAL:HG13	2.20	0.41
1:A:211:HIS:CD2	1:A:386:LEU:HD21	2.55	0.41
1:A:283:ILE:HG23	1:A:284:TYR:N	2.35	0.41
1:A:206:ILE:N	1:A:226:LEU:HD13	2.35	0.41
1:A:363:GLU:O	1:A:367:GLY:N	2.52	0.41
1:A:337:ASN:C	1:A:339:LYS:H	2.23	0.41
1:A:19:LYS:HD3	1:A:146:ASN:O	2.19	0.41
1:A:284:TYR:CE2	1:A:323:LYS:HB3	2.55	0.41
1:A:466:LYS:HD3	1:A:466:LYS:HA	1.83	0.41
1:A:296:ARG:NH2	1:A:331:LYS:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:CYS:HB3	1:A:395:LEU:O	2.20	0.41
1:A:420:ASP:HA	1:A:421:PRO:HD2	1.92	0.41
1:A:392:ARG:HG3	1:A:397:CYS:HB2	2.02	0.41
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.85	0.41
1:A:34:TYR:OH	1:A:133:THR:HG21	2.21	0.41
1:B:68:LYS:HB2	1:B:230:TYR:CE2	2.55	0.41
1:A:450:LEU:C	1:A:452:GLU:N	2.74	0.41
1:A:88:ARG:HH11	1:A:94:ASP:H	1.65	0.41
1:A:138:ASP:HA	1:A:139:PRO:HD2	1.85	0.41
1:A:179:THR:HG21	1:A:375:ILE:N	2.24	0.41
1:B:156:TRP:CD2	1:B:157:TYR:N	2.89	0.41
1:B:388:GLN:O	1:B:389:LYS:HB2	2.20	0.41
1:B:433:HIS:HB2	1:B:441:VAL:HG12	2.02	0.41
1:A:364:ILE:O	1:A:368:MET:HG3	2.21	0.41
1:A:413:VAL:CG1	1:A:414:PHE:N	2.84	0.41
1:A:89:GLU:OE2	1:B:238:PRO:HD3	2.21	0.41
1:A:415:LYS:O	1:A:424:ARG:HA	2.20	0.41
1:A:169:LYS:HG2	1:A:186:LEU:HD11	2.03	0.41
1:A:251:THR:HB	1:B:413:VAL:HG13	2.03	0.41
1:B:277:VAL:CG1	1:B:311:ARG:CZ	2.98	0.41
1:A:173:ALA:O	1:A:174:LYS:C	2.58	0.41
1:B:13:LEU:HD23	1:B:87:TYR:CZ	2.56	0.41
1:B:116:VAL:HB	1:B:462:PHE:HB3	2.03	0.41
1:A:372:LYS:N	1:A:372:LYS:HD2	2.36	0.41
1:B:182:ASN:ND2	1:B:184:ASP:OD2	2.54	0.41
1:A:237:VAL:HG23	1:B:89:GLU:CG	2.50	0.41
1:B:281:TYR:O	1:B:282:ASP:C	2.60	0.41
1:B:249:THR:C	1:B:250:ILE:HD12	2.41	0.41
1:A:420:ASP:OD1	1:A:420:ASP:O	2.39	0.40
1:A:156:TRP:HB2	1:A:397:CYS:SG	2.61	0.40
1:A:237:VAL:HG13	1:A:238:PRO:HD2	2.03	0.40
1:B:169:LYS:CG	1:B:482:LEU:HD11	2.50	0.40
1:A:118:ALA:HA	1:A:458:LEU:HD22	2.02	0.40
3:A:1009:HOH:O	1:B:158:PRO:HD3	2.20	0.40
1:B:23:TYR:CZ	1:B:24:LYS:NZ	2.87	0.40
1:A:332:PHE:N	1:A:332:PHE:CD1	2.89	0.40
1:A:233:THR:HG22	1:A:233:THR:O	2.20	0.40
1:A:435:THR:HB	1:A:436:PRO:HD2	2.04	0.40
1:B:23:TYR:CE1	1:B:24:LYS:HB3	2.57	0.40
1:A:235:ASP:OD2	1:A:474:ASP:OD2	2.38	0.40
1:A:432:LEU:HD13	1:A:432:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HA	1:A:147:TRP:HZ3	1.87	0.40
1:B:311:ARG:HB2	1:B:351:ILE:CG2	2.51	0.40
1:B:326:ASP:CG	1:B:330:LYS:HE2	2.41	0.40
1:B:417:PRO:HG3	1:B:423:LYS:HD2	2.02	0.40
1:B:295:LEU:O	1:B:296:ARG:C	2.60	0.40
1:B:298:LEU:O	1:B:302:ARG:HG3	2.21	0.40
1:A:311:ARG:HD2	1:A:351:ILE:HD11	2.04	0.40
1:A:193:PHE:O	1:A:195:TYR:N	2.53	0.40
1:A:325:LEU:HB3	1:A:373:TRP:CE2	2.57	0.40
1:B:396:ASN:HD22	1:B:396:ASN:HA	1.58	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	459/491 (94%)	387 (84%)	60 (13%)	12 (3%)	7	26
1	B	459/491 (94%)	399 (87%)	47 (10%)	13 (3%)	6	24
All	All	918/982 (94%)	786 (86%)	107 (12%)	25 (3%)	6	25

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASP
1	A	346	PRO
1	B	282	ASP
1	B	394	LEU
1	B	419	ALA
1	B	439	THR
1	A	179	THR
1	A	194	GLY

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Mol	Chain	Res	Type
1	A	313	ASP
1	A	338	SER
1	A	439	THR
1	B	395	LEU
1	B	451	GLU
1	A	451	GLU
1	A	452	GLU
1	B	333	PRO
1	B	450	LEU
1	B	93	ASP
1	B	389	LYS
1	B	29	ASN
1	A	40	ARG
1	A	238	PRO
1	B	40	ARG
1	A	237	VAL
1	B	236	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	408/431 (95%)	378 (93%)	30 (7%)	17 44
1	B	408/431 (95%)	380 (93%)	28 (7%)	19 48
All	All	816/862 (95%)	758 (93%)	58 (7%)	18 47

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	LEU
1	A	18	TYR
1	A	23	TYR
1	A	40	ARG
1	A	94	ASP

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Mol	Chain	Res	Type
1	A	119	VAL
1	A	144	LEU
1	A	182	ASN
1	A	184	ASP
1	A	190	LEU
1	A	195	TYR
1	A	196	ARG
1	A	219	ASP
1	A	233	THR
1	A	234	LYS
1	A	260	ASP
1	A	271	SER
1	A	277	VAL
1	A	314	SER
1	A	316	ASN
1	A	334	VAL
1	A	337	ASN
1	A	342	LYS
1	A	365	VAL
1	A	390	LEU
1	A	392	ARG
1	A	393	ASP
1	A	422	ASN
1	A	451	GLU
1	B	12	LEU
1	B	18	TYR
1	B	67	ASN
1	B	71	LYS
1	B	91	PHE
1	B	93	ASP
1	B	94	ASP
1	B	99	ARG
1	B	102	ASN
1	B	119	VAL
1	B	144	LEU
1	B	150	THR
1	B	186	LEU
1	B	190	LEU
1	B	195	TYR
1	B	199	SER
1	B	219	ASP
1	B	277	VAL

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Mol	Chain	Res	Type
1	B	280	SER
1	B	304	THR
1	B	334	VAL
1	B	337	ASN
1	B	365	VAL
1	B	386	LEU
1	B	396	ASN
1	B	400	LYS
1	B	432	LEU
1	B	483	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	111	HIS
1	A	146	ASN
1	A	164	ASN
1	A	168	GLN
1	A	182	ASN
1	A	211	HIS
1	A	214	ASN
1	A	247	HIS
1	A	337	ASN
1	A	370	GLN
1	A	396	ASN
1	A	407	ASN
1	A	412	ASN
1	A	422	ASN
1	B	67	ASN
1	B	90	HIS
1	B	97	ASN
1	B	102	ASN
1	B	111	HIS
1	B	164	ASN
1	B	182	ASN
1	B	191	HIS
1	B	201	GLN
1	B	211	HIS
1	B	214	ASN
1	B	337	ASN
1	B	370	GLN

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Mol	Chain	Res	Type
1	B	396	ASN
1	B	481	GLN

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NMN	A	1001	-	20,23,23	2.35	7 (35%)	26,34,34	1.39	5 (19%)
2	NMN	B	1002	-	20,23,23	2.53	7 (35%)	26,34,34	1.44	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMN	A	1001	-	-	0/10/30/30	0/2/2/2
2	NMN	B	1002	-	-	0/10/30/30	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	NMN	P-O1P	-2.64	1.45	1.54
2	A	1001	NMN	P-O1P	-2.45	1.45	1.54
2	A	1001	NMN	C6-C5	2.01	1.43	1.38
2	A	1001	NMN	C3R-C4R	2.19	1.58	1.53
2	B	1002	NMN	C6-C5	2.31	1.43	1.38
2	B	1002	NMN	C3R-C4R	2.58	1.60	1.53
2	A	1001	NMN	C5-C4	2.84	1.44	1.38
2	B	1002	NMN	C5-C4	3.00	1.45	1.38
2	A	1001	NMN	O4R-C1R	4.17	1.46	1.41
2	A	1001	NMN	C6-N1	4.17	1.46	1.35
2	B	1002	NMN	C6-N1	4.45	1.47	1.35
2	B	1002	NMN	O4R-C1R	4.79	1.47	1.41
2	A	1001	NMN	C4-C3	6.25	1.50	1.39
2	B	1002	NMN	C4-C3	6.35	1.50	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1002	NMN	O7-C7-C3	-3.31	115.97	119.59
2	A	1001	NMN	O7-C7-C3	-3.02	116.29	119.59
2	B	1002	NMN	O2P-P-O1P	2.13	115.48	107.38
2	A	1001	NMN	O2P-P-O5R	2.20	112.90	106.56
2	A	1001	NMN	O2P-P-O1P	2.21	115.78	107.38
2	B	1002	NMN	O2P-P-O5R	2.35	113.34	106.56
2	B	1002	NMN	C2-C3-C4	2.35	120.91	118.29
2	A	1001	NMN	C2-C3-C4	2.43	120.99	118.29
2	A	1001	NMN	C3-C7-N7	2.94	121.04	117.82
2	B	1002	NMN	C3-C7-N7	3.45	121.59	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NMN	5	0
2	B	1002	NMN	3	0

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	463/491 (94%)	-0.12	5 (1%)	82 80	10, 27, 45, 58	0
1	B	463/491 (94%)	-0.13	9 (1%)	70 66	11, 27, 46, 67	0
All	All	926/982 (94%)	-0.12	14 (1%)	76 74	10, 27, 45, 67	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	VAL	4.6
1	B	236	PRO	4.3
1	A	89	GLU	3.1
1	B	240	TYR	2.9
1	A	451	GLU	2.7
1	B	105	LEU	2.6
1	B	235	ASP	2.5
1	A	233	THR	2.3
1	B	106	GLU	2.3
1	B	109	ASP	2.3
1	A	314	SER	2.2
1	A	271	SER	2.2
1	B	103	TYR	2.1
1	B	76	THR	2.0

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NMN	B	1002	22/22	0.96	0.17	0.08	19,22,25,26	0
2	NMN	A	1001	22/22	0.96	0.18	-0.29	20,29,31,32	0

6.5 Other polymers

There are no such residues in this entry.