Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:17 AM GMT

PDB ID	:	2WK5
Title	:	STRUCTURAL FEATURES OF NATIVE HUMAN THYMIDINE PHOSPHORYLASE AND IN COMPLEX WITH 5-IODOURACIL
Authors	:	Mitsiki, E.; Papageorgiou, A.C.; Iyer, S.; Thiyagarajan, N.; Prior, S.H.; Sleep, D.; Finnis, C.; Acharya, K.R.
Deposited on	:	2009-06-05
Resolution	:	2.99 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:

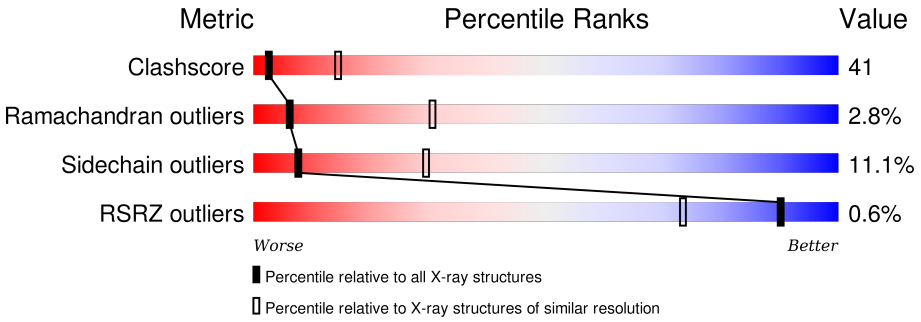
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	482	46% 42% 5% 7%
1	B	482	% 45% 41% 8% 7%
1	C	482	% 37% 47% 7% 8%
1	D	482	% 38% 47% 7% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	1481	-	X	-	X

2 Entry composition

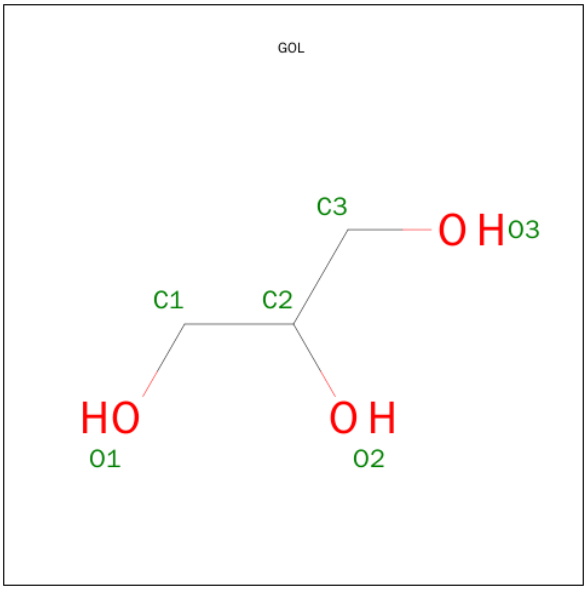
There are 3 unique types of molecules in this entry. The entry contains 13034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDINE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	1
			3271	2043	600	612	16			
1	B	448	Total	C	N	O	S	0	0	1
			3262	2039	596	611	16			
1	C	445	Total	C	N	O	S	0	0	1
			3243	2023	596	608	16			
1	D	445	Total	C	N	O	S	0	0	1
			3234	2020	592	606	16			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

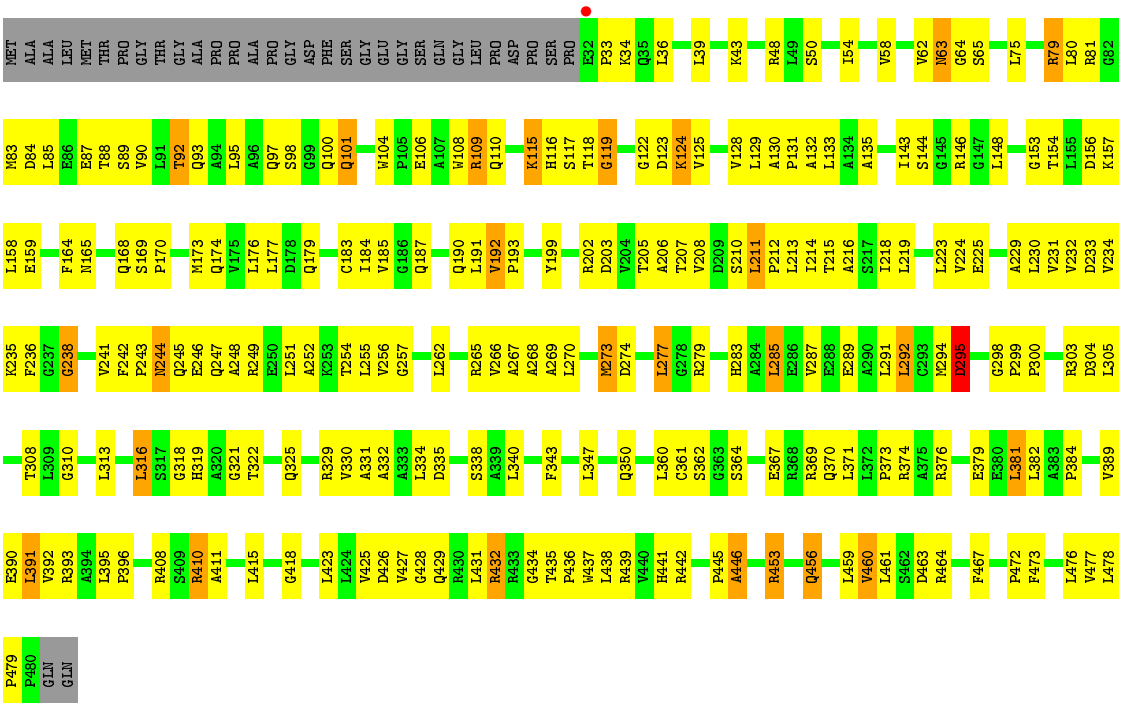
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total O 6 6	0	0
3	B	7	Total O 7 7	0	0
3	C	2	Total O 2 2	0	0
3	D	3	Total O 3 3	0	0

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.

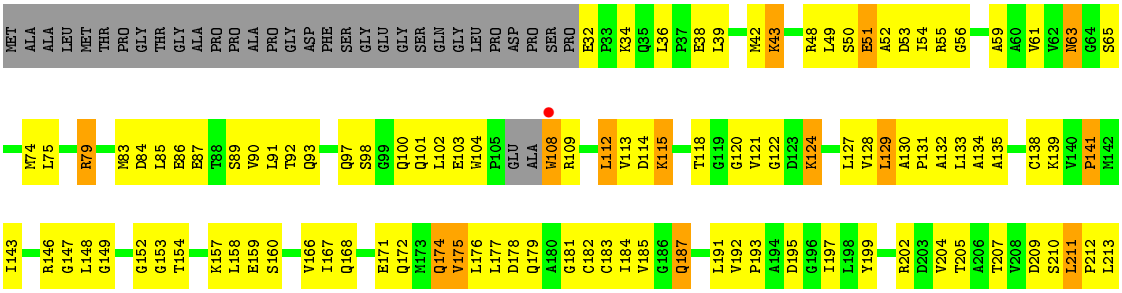
- Molecule 1: THYMIDINE PHOSPHORYLASE

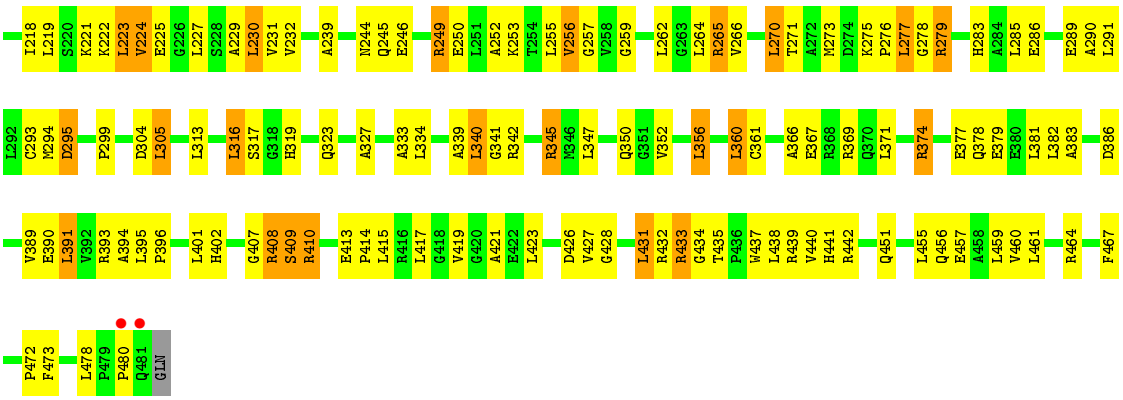
Chain A:



- Molecule 1: THYMIDINE PHOSPHORYLASE

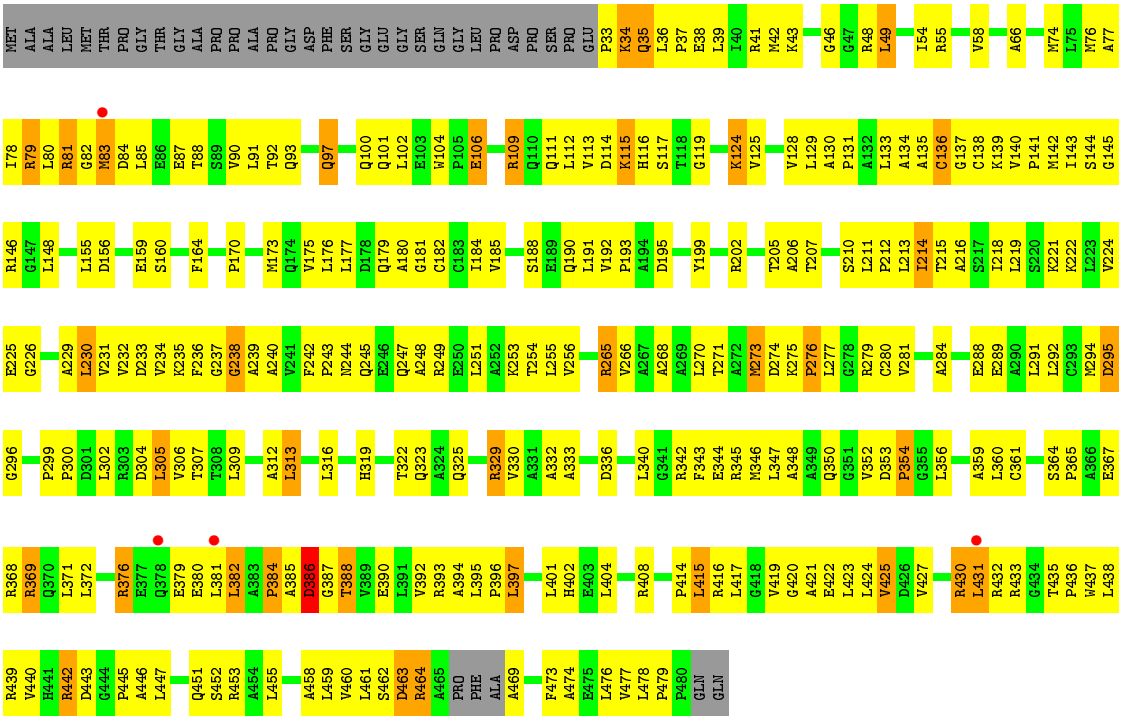
Chain B:





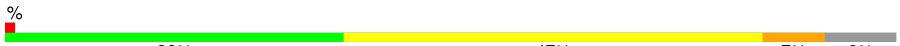
• Molecule 1: THYMIDINE PHOSPHORYLASE

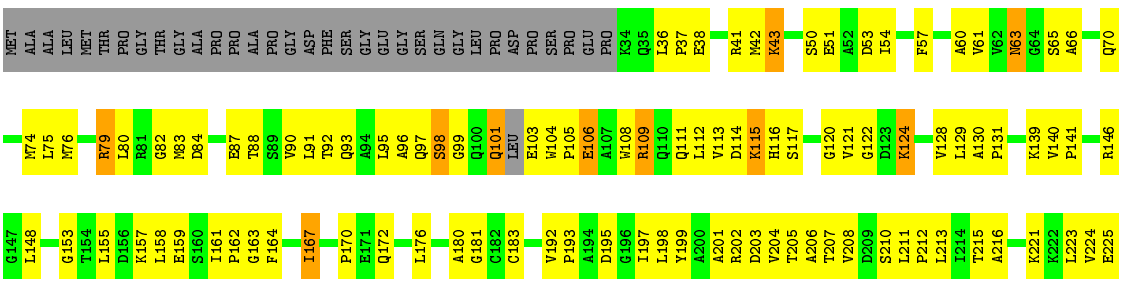
Chain C:

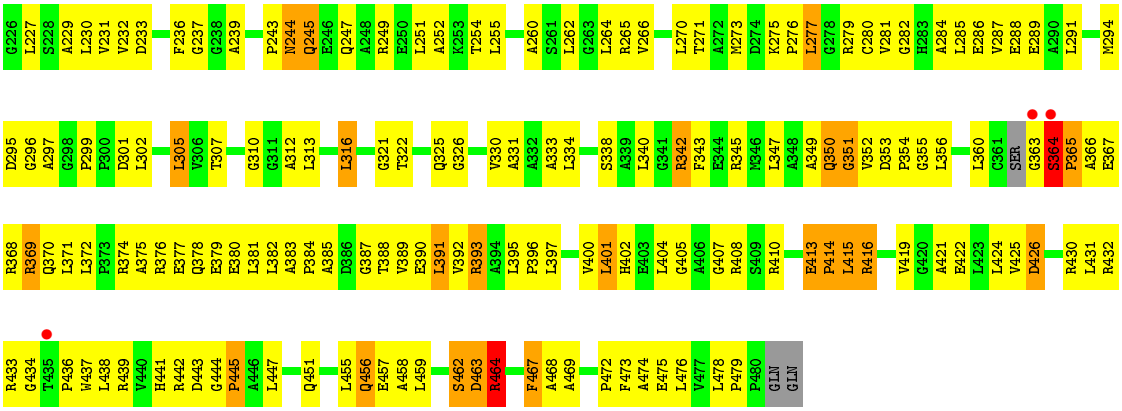


• Molecule 1: THYMIDINE PHOSPHORYLASE

Chain D:






G226 L227 S228 A229 L230 V231 V232 D233 F236 G237 G238 A239 P243 N244 Q245 E246 Q247 A248 R249 E250 L251 A252 K253 T254 L255 A260 S261 L262 G263 L264 R265 V266 L270 T271 A272 H273 D274 K275 P276 L277 G278 R279 C280 V281 G282 H283 A284 L285 E286 V287 E288 E289 A290 L291 M294
D295 G296 A297 G298 P299 P300 D301 L302 L305 V306 T307 G310 G311 A312 L313 L316 G321 T322 Q325 G326 V330 A331 A332 A333 L334 S338 A339 L340 G341 R342 F343 E344 R345 N346 L347 A348 A349 Q350 G351 V352 D353 P354 G355 L356 L360 C361 SER G363 S364 P365 A366 E367
R368 R369 Q370 L371 L372 P373 R374 A375 R376 E377 Q378 E379 E380 I381 I382 A383 P384 A385 D386 G387 T388 V389 E390 I391 V392 R393 A394 L395 P396 L397 V400 L401 H402 E403 L404 G405 A406 G407 R408 S409 R410 E413 P414 L415 R416 V419 G420 A421 E422 L423 L424 V425 D426 R430 L431 R432
R433 G434 T435 P436 W437 L438 R439 V440 H441 R442 D443 G444 P445 A446 L447 Q451 L455 Q456 E457 A458 L459 S462 D463 R464 F467 A468 A469 P472 F473 A474 E475 L476 V477 L478 P479 P480 GLN GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.53Å 77.19Å 100.88Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	42.61 – 2.99 42.61 – 2.99	Depositor EDS
% Data completeness (in resolution range)	85.2 (42.61-2.99) 85.3 (42.61-2.99)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.207 , 0.284 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.3	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 30100 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13034	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 36.47 % 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 4.9739e-04.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: GOL

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	0.40	0/3318	0.68	0/4502
1	B	0.40	0/3309	0.68	0/4490
1	C	0.35	0/3287	0.65	0/4456
1	D	0.38	0/3278	0.66	1/4446 (0.0%)
All	All	0.38	0/13192	0.67	1/17894 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	364	SER	C-N-CD	-6.36	106.62	120.60

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	3271	0	3364	208	0
1	B	3262	0	3352	259	0
1	C	3243	0	3341	327	0
1	D	3234	0	3311	296	0
2	B	6	0	4	0	0
3	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	13034	0	13372	1085	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 41.

All (1085) 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:D:363:GLY:O	1:D:368:ARG:NH1	1.57	1.37
1:B:408:ARG:HG3	1:B:413:GLU:CG	1.65	1.26
1:B:408:ARG:HG3	1:B:413:GLU:HG2	1.22	1.20
1:B:102:LEU:HD22	1:B:104:TRP:CZ2	1.78	1.18
1:C:386:ASP:HB2	1:C:432:ARG:HA	1.30	1.14
1:D:364:SER:O	1:D:368:ARG:NH1	1.80	1.13
1:B:283:HIS:NE2	1:B:415:LEU:HD23	1.64	1.12
1:C:92:THR:HG22	1:C:216:ALA:HA	1.29	1.10
1:C:464:ARG:HH11	1:C:464:ARG:HG3	1.15	1.07
1:D:164:PHE:CZ	1:D:350:GLN:OE1	2.07	1.07
1:B:283:HIS:CE1	1:B:415:LEU:HD23	1.91	1.05
1:A:100:GLN:HE21	1:A:190:GLN:HB3	1.17	1.02
1:A:426:ASP:H	1:A:429:GLN:HE21	1.07	1.02
1:C:230:LEU:HD12	1:C:266:VAL:HG12	1.38	1.00
1:D:245:GLN:NE2	1:D:245:GLN:H	1.60	1.00
1:C:369:ARG:HH11	1:C:369:ARG:HB2	1.24	0.99
1:C:386:ASP:HB2	1:C:432:ARG:CA	1.92	0.99
1:D:163:GLY:O	1:D:351:GLY:O	1.81	0.98
1:C:464:ARG:HH11	1:C:464:ARG:CG	1.76	0.98
1:A:285:LEU:H	1:A:285:LEU:HD12	1.28	0.96
1:B:408:ARG:HG3	1:B:413:GLU:HG3	1.46	0.95
1:C:211:LEU:HD11	1:C:254:THR:HG21	1.48	0.95
1:B:187:GLN:H	1:B:187:GLN:HE21	0.98	0.95
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.49	0.95
1:D:456:GLN:HE21	1:D:456:GLN:HA	1.33	0.93
1:D:322:THR:HG23	1:D:325:GLN:H	1.33	0.93
1:B:187:GLN:H	1:B:187:GLN:NE2	1.67	0.92
1:A:322:THR:HG22	1:A:325:GLN:HG3	1.48	0.92
1:D:347:LEU:O	1:D:352:VAL:HG23	1.71	0.91
1:A:223:LEU:HD11	1:A:262:LEU:HD13	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:LYS:HG3	1:D:302:LEU:HD21	1.50	0.91
1:D:141:PRO:HA	1:D:183:CYS:SG	2.11	0.91
1:B:381:LEU:HD12	1:B:438:LEU:HD23	1.51	0.91
1:C:229:ALA:HB1	1:C:316:LEU:HD12	1.51	0.91
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.53	0.90
1:D:365:PRO:O	1:D:368:ARG:N	2.04	0.90
1:C:386:ASP:CB	1:C:432:ARG:HA	2.02	0.90
1:B:279:ARG:HG2	1:B:423:LEU:O	1.73	0.89
1:D:356:LEU:HD22	1:D:371:LEU:HD23	1.54	0.89
1:D:101:GLN:HE21	1:D:224:VAL:HG22	1.37	0.89
1:C:101:GLN:HE21	1:C:224:VAL:HG22	1.36	0.89
1:C:210:SER:HB3	1:C:213:LEU:HB2	1.55	0.89
1:A:79:ARG:O	1:A:79:ARG:HD3	1.72	0.88
1:C:33:PRO:O	1:C:34:LYS:HG3	1.73	0.88
1:A:229:ALA:HB1	1:A:316:LEU:HD12	1.53	0.88
1:C:55:ARG:HH12	1:C:97:GLN:HE22	1.16	0.88
1:B:402:HIS:NE2	1:B:409:SER:HB2	1.89	0.88
1:B:102:LEU:HD22	1:B:104:TRP:CE2	2.09	0.87
1:C:55:ARG:NH1	1:C:97:GLN:HE22	1.73	0.87
1:B:381:LEU:HB3	1:B:456:GLN:HE22	1.38	0.86
1:C:48:ARG:HD2	1:C:84:ASP:OD2	1.75	0.86
1:D:289:GLU:OE1	1:D:299:PRO:HG2	1.76	0.86
1:D:93:GLN:O	1:D:97:GLN:HG2	1.75	0.86
1:C:170:PRO:HA	1:C:173:MET:HE3	1.56	0.86
1:A:63:ASN:HD22	1:A:64:GLY:N	1.72	0.86
1:C:453:ARG:HH11	1:C:453:ARG:HB3	1.41	0.85
1:D:162:PRO:O	1:D:352:VAL:HG13	1.76	0.85
1:B:109:ARG:HA	1:B:112:LEU:HD12	1.59	0.85
1:B:408:ARG:CG	1:B:413:GLU:HG2	2.06	0.84
1:C:453:ARG:NH1	1:C:453:ARG:HB3	1.92	0.84
1:A:100:GLN:NE2	1:A:190:GLN:HB3	1.91	0.84
1:C:271:THR:HG21	1:C:305:LEU:HD21	1.58	0.84
1:B:366:ALA:CB	1:D:99:GLY:HA2	2.07	0.84
1:A:118:THR:OG1	1:A:119:GLY:N	2.09	0.84
1:B:374:ARG:CG	1:B:374:ARG:HH11	1.89	0.83
1:D:291:LEU:HD13	1:D:368:ARG:HE	1.43	0.83
1:B:249:ARG:HB3	1:B:249:ARG:HH11	1.41	0.83
1:B:431:LEU:HD21	1:B:435:THR:HB	1.59	0.83
1:C:173:MET:HA	1:C:176:LEU:HD12	1.60	0.83
1:B:285:LEU:HD21	1:B:369:ARG:NH2	1.94	0.82
1:C:393:ARG:CB	1:C:458:ALA:HA	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:O	1:A:119:GLY:O	1.98	0.82
1:C:386:ASP:HB2	1:C:433:ARG:N	1.94	0.82
1:B:102:LEU:CD2	1:B:104:TRP:CZ2	2.63	0.81
1:C:393:ARG:HG3	1:C:396:PRO:CD	2.10	0.81
1:D:422:GLU:HB2	1:D:439:ARG:HB3	1.63	0.81
1:D:163:GLY:C	1:D:351:GLY:O	2.20	0.80
1:B:374:ARG:HG3	1:B:374:ARG:HH11	1.46	0.80
1:D:463:ASP:O	1:D:464:ARG:O	1.99	0.80
1:A:75:LEU:HB3	1:A:207:THR:HG21	1.63	0.80
1:A:88:THR:O	1:A:92:THR:HG22	1.80	0.80
1:D:79:ARG:HG3	1:D:207:THR:HA	1.64	0.80
1:D:84:ASP:OD2	1:D:87:GLU:HG3	1.82	0.80
1:C:416:ARG:NH1	1:C:443:ASP:HB3	1.96	0.80
1:C:92:THR:HG22	1:C:216:ALA:CA	2.09	0.80
1:B:175:VAL:HG22	1:B:179:GLN:HE21	1.46	0.80
1:C:395:LEU:HB3	1:C:396:PRO:HD3	1.63	0.79
1:B:63:ASN:C	1:B:63:ASN:HD22	1.85	0.79
1:B:374:ARG:HG3	1:B:374:ARG:NH1	1.97	0.79
1:D:395:LEU:HB3	1:D:396:PRO:HD3	1.65	0.79
1:C:397:LEU:O	1:C:401:LEU:HD23	1.83	0.79
1:C:478:LEU:HD12	1:C:479:PRO:HD2	1.64	0.79
1:B:395:LEU:HB3	1:B:396:PRO:HD3	1.64	0.79
1:A:428:GLY:HA2	1:A:467:PHE:CE2	2.18	0.78
1:B:166:VAL:HG23	1:B:167:ILE:HD12	1.66	0.78
1:B:49:LEU:HB2	1:B:54:ILE:HD11	1.64	0.78
1:C:294:MET:HB3	1:C:340:LEU:HB2	1.64	0.78
1:D:463:ASP:O	1:D:464:ARG:C	2.16	0.78
1:C:249:ARG:HH12	1:C:253:LYS:HE2	1.47	0.78
1:A:104:TRP:H	1:A:109:ARG:HH12	1.30	0.78
1:B:283:HIS:CE1	1:B:415:LEU:CD2	2.67	0.78
1:C:173:MET:HE2	1:C:191:LEU:HD11	1.63	0.77
1:B:366:ALA:HB1	1:D:99:GLY:HA2	1.66	0.77
1:B:112:LEU:HD23	1:B:139:LYS:HB3	1.65	0.77
1:B:381:LEU:HB3	1:B:456:GLN:NE2	1.98	0.77
1:B:139:LYS:HG3	1:B:177:LEU:HD13	1.66	0.77
1:B:239:ALA:HB3	1:B:273:MET:HG3	1.67	0.77
1:C:274:ASP:O	1:C:394:ALA:HB3	1.84	0.77
1:C:427:VAL:CG1	1:C:469:ALA:HB2	2.16	0.76
1:B:79:ARG:HG3	1:B:207:THR:HG22	1.68	0.76
1:A:453:ARG:HB3	1:B:179:GLN:OE1	1.84	0.76
1:D:245:GLN:CD	1:D:245:GLN:H	1.88	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:181:GLY:HA2	1.86	0.76
1:D:291:LEU:HB3	1:D:368:ARG:HH21	1.52	0.76
1:C:416:ARG:HH11	1:C:443:ASP:HB3	1.48	0.75
1:D:390:GLU:CG	1:D:462:SER:OG	2.34	0.75
1:B:187:GLN:HE21	1:B:187:GLN:N	1.79	0.75
1:B:381:LEU:HD13	1:B:456:GLN:HE21	1.52	0.75
1:C:386:ASP:HB2	1:C:433:ARG:H	1.48	0.75
1:B:431:LEU:HD23	1:B:432:ARG:H	1.50	0.75
1:B:102:LEU:CD1	1:B:225:GLU:HA	2.17	0.75
1:B:249:ARG:HH11	1:B:249:ARG:CB	1.99	0.74
1:B:283:HIS:NE2	1:B:415:LEU:CD2	2.48	0.74
1:C:102:LEU:HD21	1:C:173:MET:HE3	1.69	0.74
1:B:63:ASN:ND2	1:B:65:SER:H	1.86	0.74
1:D:405:GLY:HA3	1:D:416:ARG:HG3	1.70	0.74
1:B:259:GLY:HA3	1:B:266:VAL:HG21	1.69	0.74
1:A:143:ILE:HG13	1:A:225:GLU:OE1	1.88	0.74
1:A:294:MET:O	1:A:295:ASP:O	2.06	0.74
1:C:442:ARG:NH2	1:C:446:ALA:HA	2.03	0.74
1:A:63:ASN:ND2	1:A:65:SER:H	1.85	0.74
1:B:146:ARG:NH1	1:B:159:GLU:OE2	2.20	0.74
1:D:230:LEU:HD12	1:D:266:VAL:HG13	1.68	0.73
1:A:92:THR:HB	1:A:216:ALA:HA	1.69	0.73
1:C:386:ASP:CB	1:C:433:ARG:H	2.00	0.73
1:C:393:ARG:HB2	1:C:458:ALA:HA	1.68	0.73
1:B:431:LEU:CD2	1:B:435:THR:HB	2.19	0.73
1:D:161:ILE:HD11	1:D:287:VAL:HG11	1.71	0.72
1:B:184:ILE:H	1:B:350:GLN:HE22	1.37	0.72
1:A:63:ASN:C	1:A:63:ASN:HD22	1.91	0.72
1:C:401:LEU:HD13	1:C:404:LEU:HD12	1.70	0.72
1:B:49:LEU:HB2	1:B:54:ILE:CD1	2.18	0.72
1:A:79:ARG:HB2	1:A:207:THR:HG23	1.70	0.72
1:C:88:THR:O	1:C:92:THR:HG23	1.90	0.72
1:A:176:LEU:HD21	1:A:350:GLN:HG3	1.70	0.72
1:A:392:VAL:HG21	1:A:423:LEU:HD11	1.71	0.72
1:C:381:LEU:O	1:C:437:TRP:NE1	2.23	0.71
1:D:356:LEU:HD13	1:D:356:LEU:O	1.90	0.71
1:D:456:GLN:NE2	1:D:456:GLN:HA	2.05	0.71
1:B:377:GLU:HB3	1:B:442:ARG:HH22	1.55	0.71
1:D:239:ALA:HB3	1:D:273:MET:HG3	1.72	0.71
1:D:167:ILE:HD12	1:D:167:ILE:H	1.53	0.71
1:D:390:GLU:OE2	1:D:464:ARG:CD	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:NE	1:A:415:LEU:HD13	2.05	0.71
1:C:173:MET:CE	1:C:191:LEU:HD11	2.20	0.71
1:C:55:ARG:HH12	1:C:97:GLN:NE2	1.88	0.71
1:A:410:ARG:O	1:A:410:ARG:HG2	1.91	0.71
1:A:234:VAL:HB	1:A:270:LEU:HD23	1.73	0.71
1:C:401:LEU:HA	1:C:404:LEU:HD12	1.71	0.71
1:B:249:ARG:HB3	1:B:249:ARG:NH1	2.04	0.70
1:C:390:GLU:HG3	1:C:462:SER:HB3	1.71	0.70
1:C:268:ALA:HB3	1:C:477:VAL:HB	1.70	0.70
1:C:393:ARG:HH11	1:C:393:ARG:HG2	1.55	0.70
1:D:96:ALA:O	1:D:101:GLN:NE2	2.20	0.70
1:A:211:LEU:HD21	1:A:254:THR:HG21	1.73	0.70
1:B:135:ALA:HA	1:B:342:ARG:NE	2.06	0.70
1:B:175:VAL:HG22	1:B:179:GLN:NE2	2.05	0.70
1:C:422:GLU:OE1	1:C:439:ARG:HD2	1.91	0.70
1:D:93:GLN:HB3	1:D:97:GLN:HE21	1.55	0.70
1:D:60:ALA:HA	1:D:63:ASN:HD21	1.54	0.70
1:B:130:ALA:HB3	1:B:131:PRO:HD3	1.72	0.70
1:D:244:ASN:HB3	1:D:247:GLN:HB3	1.72	0.70
1:B:408:ARG:CG	1:B:413:GLU:CG	2.58	0.70
1:B:154:THR:HA	1:B:157:LYS:HD2	1.74	0.70
1:C:289:GLU:OE2	1:C:299:PRO:HG2	1.91	0.69
1:B:408:ARG:HG2	1:B:408:ARG:O	1.92	0.69
1:D:101:GLN:NE2	1:D:224:VAL:HG22	2.07	0.69
1:C:381:LEU:O	1:C:437:TRP:CD1	2.45	0.69
1:C:459:LEU:HD22	1:C:461:LEU:HG	1.73	0.69
1:C:392:VAL:HA	1:C:458:ALA:O	1.92	0.69
1:C:369:ARG:HB2	1:C:369:ARG:NH1	2.04	0.69
1:D:463:ASP:C	1:D:464:ARG:O	2.28	0.69
1:C:111:GLN:HE21	1:C:319:HIS:CE1	2.10	0.69
1:B:205:THR:O	1:B:205:THR:HG22	1.92	0.69
1:B:408:ARG:HB3	1:B:415:LEU:HD11	1.73	0.69
1:C:464:ARG:CG	1:C:464:ARG:NH1	2.45	0.69
1:D:379:GLU:OE1	1:D:447:LEU:HG	1.93	0.69
1:A:445:PRO:O	1:A:446:ALA:HB2	1.93	0.69
1:A:205:THR:HG22	1:A:207:THR:OG1	1.93	0.69
1:D:390:GLU:HG3	1:D:462:SER:OG	1.93	0.69
1:D:202:ARG:HD2	1:D:213:LEU:HD22	1.73	0.69
1:D:416:ARG:NH1	1:D:443:ASP:OD1	2.24	0.69
1:A:426:ASP:O	1:A:429:GLN:HG2	1.92	0.68
1:A:123:ASP:OD2	1:A:277:LEU:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ALA:HA	1:C:342:ARG:NH1	2.08	0.68
1:A:322:THR:CG2	1:A:325:GLN:HG3	2.23	0.68
1:C:249:ARG:NH1	1:C:253:LYS:HE2	2.09	0.68
1:C:130:ALA:HB3	1:C:131:PRO:HD3	1.76	0.68
1:A:235:LYS:HE3	1:A:273:MET:HG2	1.75	0.68
1:C:101:GLN:NE2	1:C:224:VAL:HG22	2.09	0.68
1:B:172:GLN:O	1:B:176:LEU:HD23	1.93	0.68
1:D:347:LEU:O	1:D:352:VAL:CG2	2.42	0.68
1:A:437:TRP:CE3	1:A:459:LEU:HD23	2.28	0.68
1:B:378:GLN:NE2	1:B:439:ARG:HD3	2.09	0.68
1:D:223:LEU:HD11	1:D:262:LEU:HB3	1.75	0.67
1:A:370:GLN:HG2	1:A:374:ARG:NH1	2.09	0.67
1:D:205:THR:O	1:D:206:ALA:HB3	1.93	0.67
1:C:211:LEU:CD1	1:C:254:THR:HG21	2.23	0.67
1:C:386:ASP:CB	1:C:433:ARG:N	2.58	0.67
1:C:249:ARG:HH12	1:C:253:LYS:CE	2.07	0.67
1:D:36:LEU:HD11	1:D:57:PHE:HD1	1.59	0.67
1:A:124:LYS:H	1:A:124:LYS:HD2	1.58	0.67
1:A:391:LEU:HA	1:A:427:VAL:HG22	1.77	0.66
1:D:326:GLY:O	1:D:330:VAL:HG23	1.95	0.66
1:D:106:GLU:HA	1:D:109:ARG:HH11	1.60	0.66
1:C:230:LEU:HD12	1:C:266:VAL:CG1	2.21	0.66
1:A:442:ARG:CZ	1:A:446:ALA:HA	2.25	0.66
1:D:161:ILE:HG21	1:D:347:LEU:HD22	1.78	0.66
1:C:393:ARG:HG3	1:C:396:PRO:CG	2.25	0.66
1:A:285:LEU:CD1	1:A:285:LEU:H	2.05	0.66
1:C:133:LEU:HD11	1:C:313:LEU:HD12	1.78	0.66
1:D:192:VAL:HG13	1:D:224:VAL:HG21	1.77	0.66
1:C:343:PHE:CE2	1:C:347:LEU:HD11	2.31	0.66
1:D:210:SER:HB3	1:D:213:LEU:HB2	1.78	0.66
1:C:54:ILE:O	1:C:58:VAL:HG23	1.95	0.66
1:D:106:GLU:HA	1:D:109:ARG:HD3	1.78	0.66
1:C:478:LEU:CD1	1:C:479:PRO:HD2	2.26	0.66
1:C:393:ARG:HB3	1:C:458:ALA:HA	1.78	0.65
1:D:270:LEU:HB2	1:D:474:ALA:HB3	1.78	0.65
1:C:464:ARG:HG3	1:C:464:ARG:NH1	1.97	0.65
1:C:427:VAL:HG11	1:C:469:ALA:HB2	1.76	0.65
1:D:330:VAL:O	1:D:334:LEU:HG	1.96	0.65
1:D:365:PRO:HA	1:D:368:ARG:HD3	1.79	0.65
1:D:365:PRO:O	1:D:366:ALA:C	2.33	0.65
1:C:300:PRO:O	1:C:304:ASP:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ARG:HG2	1:C:279:ARG:HH21	1.61	0.65
1:B:55:ARG:HH12	1:B:97:GLN:HE22	1.45	0.65
1:C:83:MET:CB	1:C:87:GLU:OE2	2.45	0.65
1:D:376:ARG:HB3	1:D:443:ASP:HA	1.79	0.65
1:D:276:PRO:HG2	1:D:397:LEU:HD23	1.77	0.65
1:D:385:ALA:HA	1:D:433:ARG:HB2	1.78	0.65
1:D:390:GLU:OE2	1:D:464:ARG:HD3	1.96	0.65
1:C:422:GLU:HB3	1:C:439:ARG:HB3	1.79	0.65
1:D:390:GLU:HG2	1:D:462:SER:OG	1.96	0.65
1:B:89:SER:O	1:B:92:THR:HG22	1.97	0.65
1:D:367:GLU:OE1	1:D:371:LEU:HD11	1.97	0.65
1:B:285:LEU:CD2	1:B:369:ARG:NH2	2.59	0.65
1:A:165:ASN:HB3	1:A:168:GLN:HE22	1.61	0.65
1:D:164:PHE:HZ	1:D:350:GLN:OE1	1.77	0.65
1:C:124:LYS:H	1:C:124:LYS:HD2	1.62	0.65
1:C:55:ARG:NH1	1:C:97:GLN:NE2	2.42	0.64
1:B:408:ARG:HB3	1:B:415:LEU:CD1	2.26	0.64
1:D:230:LEU:HD13	1:D:231:VAL:N	2.12	0.64
1:A:442:ARG:NE	1:A:446:ALA:HA	2.12	0.64
1:C:393:ARG:HG3	1:C:396:PRO:HG2	1.79	0.64
1:D:88:THR:O	1:D:92:THR:HG23	1.98	0.64
1:C:388:THR:HA	1:C:430:ARG:CB	2.27	0.64
1:C:256:VAL:HG22	1:C:479:PRO:HB3	1.78	0.64
1:A:428:GLY:HA2	1:A:467:PHE:CZ	2.33	0.64
1:A:395:LEU:HB3	1:A:396:PRO:HD3	1.79	0.64
1:C:113:VAL:HB	1:C:313:LEU:HD11	1.78	0.64
1:D:60:ALA:HA	1:D:65:SER:HB3	1.80	0.64
1:A:115:LYS:HA	1:A:231:VAL:O	1.97	0.64
1:C:380:GLU:OE2	1:C:436:PRO:HB3	1.98	0.64
1:A:459:LEU:CD1	1:A:461:LEU:HG	2.28	0.64
1:D:76:MET:HE2	1:D:76:MET:O	1.98	0.63
1:B:128:VAL:HG13	1:B:294:MET:HE2	1.79	0.63
1:A:269:ALA:HB2	1:A:476:LEU:HD12	1.81	0.63
1:D:50:SER:H	1:D:53:ASP:HB2	1.62	0.63
1:D:164:PHE:N	1:D:352:VAL:HG22	2.12	0.63
1:C:322:THR:OG1	1:C:325:GLN:HB2	1.97	0.63
1:C:202:ARG:HH12	1:C:214:ILE:HG12	1.64	0.63
1:B:102:LEU:HD13	1:B:225:GLU:HA	1.79	0.63
1:C:464:ARG:CB	1:C:464:ARG:NH1	2.61	0.63
1:D:244:ASN:HD22	1:D:245:GLN:N	1.96	0.63
1:C:36:LEU:HD23	1:C:39:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLY:O	1:B:345:ARG:HD3	1.97	0.63
1:A:340:LEU:HD22	1:A:361:CYS:HB3	1.81	0.63
1:D:467:PHE:N	1:D:467:PHE:CD1	2.67	0.63
1:C:388:THR:HG23	1:C:430:ARG:HB3	1.79	0.63
1:C:386:ASP:HB2	1:C:432:ARG:C	2.19	0.63
1:B:275:LYS:HE2	1:B:276:PRO:O	1.99	0.63
1:B:183:CYS:HB2	1:B:350:GLN:NE2	2.13	0.62
1:A:392:VAL:HG21	1:A:423:LEU:CD1	2.29	0.62
1:C:54:ILE:HG21	1:C:90:VAL:HG12	1.79	0.62
1:D:390:GLU:OE2	1:D:464:ARG:HD2	1.99	0.62
1:B:442:ARG:HH21	1:B:442:ARG:HG3	1.63	0.62
1:C:115:LYS:HA	1:C:231:VAL:O	1.99	0.62
1:B:113:VAL:HG11	1:B:317:SER:HB2	1.81	0.62
1:A:329:ARG:O	1:A:332:ALA:HB3	1.99	0.62
1:B:222:LYS:HD3	1:B:225:GLU:OE2	1.98	0.62
1:C:431:LEU:HD23	1:C:431:LEU:H	1.64	0.62
1:C:381:LEU:HD11	1:C:455:LEU:HD23	1.81	0.62
1:D:193:PRO:O	1:D:197:ILE:HG12	1.99	0.62
1:D:57:PHE:O	1:D:61:VAL:HG23	2.00	0.62
1:B:98:SER:HB2	1:B:193:PRO:HD2	1.80	0.62
1:D:93:GLN:HE21	1:D:262:LEU:HD21	1.64	0.62
1:B:102:LEU:HD12	1:B:225:GLU:HA	1.82	0.62
1:B:43:LYS:HG3	1:B:74:MET:HE1	1.82	0.62
1:A:294:MET:O	1:A:295:ASP:C	2.37	0.62
1:A:128:VAL:O	1:A:131:PRO:HD2	2.00	0.62
1:D:93:GLN:HB3	1:D:97:GLN:NE2	2.14	0.62
1:A:408:ARG:HE	1:A:415:LEU:HD13	1.64	0.62
1:D:128:VAL:HG13	1:D:294:MET:HG2	1.82	0.61
1:B:55:ARG:HH12	1:B:97:GLN:NE2	1.97	0.61
1:C:156:ASP:O	1:C:159:GLU:HB2	2.01	0.61
1:B:381:LEU:HD13	1:B:456:GLN:NE2	2.14	0.61
1:D:371:LEU:H	1:D:371:LEU:HD12	1.65	0.61
1:C:83:MET:HB3	1:C:87:GLU:OE2	2.00	0.61
1:C:379:GLU:OE1	1:C:447:LEU:HG	2.01	0.61
1:A:129:LEU:O	1:A:133:LEU:HG	2.00	0.61
1:B:168:GLN:HG3	1:B:185:VAL:HG11	1.82	0.61
1:B:239:ALA:HB2	1:B:394:ALA:HB3	1.82	0.61
1:D:416:ARG:HB2	1:D:419:VAL:HG23	1.82	0.61
1:B:74:MET:HE2	1:B:74:MET:O	2.00	0.61
1:D:368:ARG:C	1:D:370:GLN:H	2.04	0.61
1:C:288:GLU:HG2	1:C:372:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LEU:HD13	1:D:368:ARG:NE	2.16	0.61
1:C:231:VAL:HG23	1:C:313:LEU:HD23	1.82	0.61
1:C:102:LEU:HD21	1:C:173:MET:CE	2.30	0.60
1:C:265:ARG:HD2	1:C:316:LEU:HD11	1.83	0.60
1:D:280:CYS:HB2	1:D:289:GLU:OE2	2.01	0.60
1:D:265:ARG:NH2	1:D:316:LEU:O	2.35	0.60
1:C:369:ARG:HH11	1:C:369:ARG:CB	2.09	0.60
1:D:76:MET:HE3	1:D:79:ARG:HB3	1.82	0.60
1:A:104:TRP:H	1:A:109:ARG:NH1	1.99	0.60
1:D:288:GLU:HG2	1:D:372:LEU:HD12	1.84	0.60
1:A:245:GLN:O	1:A:248:ALA:HB3	2.01	0.60
1:C:191:LEU:O	1:C:192:VAL:CG2	2.50	0.60
1:D:167:ILE:N	1:D:167:ILE:HD12	2.16	0.60
1:D:75:LEU:HD22	1:D:213:LEU:HD11	1.84	0.60
1:A:277:LEU:HD11	1:A:305:LEU:HD12	1.83	0.60
1:D:277:LEU:HD23	1:D:301:ASP:HB3	1.84	0.60
1:B:63:ASN:HD22	1:B:65:SER:H	1.50	0.60
1:D:419:VAL:HA	1:D:441:HIS:O	2.01	0.59
1:C:280:CYS:SG	1:C:289:GLU:HB2	2.41	0.59
1:B:93:GLN:HG2	1:B:97:GLN:OE1	2.02	0.59
1:D:414:PRO:O	1:D:415:LEU:HD12	2.02	0.59
1:A:48:ARG:NH1	1:A:87:GLU:HG3	2.16	0.59
1:D:98:SER:O	1:D:193:PRO:HD2	2.03	0.59
1:A:176:LEU:CD2	1:A:350:GLN:HG3	2.32	0.59
1:D:237:GLY:H	1:D:243:PRO:HA	1.67	0.59
1:B:478:LEU:O	1:B:480:PRO:HD3	2.02	0.59
1:C:160:SER:HA	1:C:417:LEU:HD13	1.84	0.59
1:C:33:PRO:O	1:C:34:LYS:CG	2.50	0.59
1:B:317:SER:OG	1:B:319:HIS:HD2	1.85	0.59
1:C:79:ARG:HG3	1:C:207:THR:HG22	1.84	0.59
1:D:368:ARG:O	1:D:370:GLN:N	2.35	0.59
1:B:408:ARG:CG	1:B:408:ARG:O	2.51	0.59
1:A:154:THR:HA	1:A:157:LYS:HD2	1.83	0.59
1:B:431:LEU:HD23	1:B:432:ARG:N	2.17	0.59
1:D:442:ARG:HD2	1:D:445:PRO:O	2.01	0.59
1:B:279:ARG:NH2	1:B:426:ASP:OD2	2.35	0.59
1:A:291:LEU:HD11	1:A:360:LEU:HD22	1.84	0.59
1:C:390:GLU:CG	1:C:462:SER:HB3	2.32	0.59
1:B:128:VAL:O	1:B:131:PRO:HD2	2.03	0.59
1:C:180:ALA:HB2	1:C:345:ARG:O	2.02	0.59
1:D:353:ASP:OD2	1:D:355:GLY:N	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:PRO:HG2	1:D:397:LEU:CD2	2.33	0.58
1:C:116:HIS:CD2	1:C:218:ILE:HG23	2.38	0.58
1:B:265:ARG:HD2	1:B:316:LEU:HD12	1.85	0.58
1:B:427:VAL:HG12	1:B:467:PHE:CZ	2.38	0.58
1:D:215:THR:HA	1:D:255:LEU:HD21	1.84	0.58
1:A:192:VAL:N	1:A:193:PRO:HD3	2.17	0.58
1:C:145:GLY:C	1:C:155:LEU:HD12	2.24	0.58
1:B:278:GLY:HA3	1:B:289:GLU:OE2	2.04	0.58
1:D:211:LEU:HG	1:D:251:LEU:HD23	1.84	0.58
1:A:101:GLN:NE2	1:A:101:GLN:N	2.51	0.58
1:C:281:VAL:HB	1:C:421:ALA:HB3	1.85	0.58
1:D:54:ILE:HG21	1:D:90:VAL:HG12	1.86	0.58
1:D:352:VAL:O	1:D:353:ASP:C	2.41	0.58
1:C:84:ASP:OD1	1:C:87:GLU:HG3	2.03	0.58
1:A:108:TRP:N	1:A:108:TRP:CD1	2.71	0.58
1:D:431:LEU:HD23	1:D:431:LEU:H	1.67	0.58
1:C:93:GLN:O	1:C:97:GLN:HG3	2.03	0.58
1:C:340:LEU:O	1:C:340:LEU:HD22	2.03	0.58
1:D:371:LEU:N	1:D:371:LEU:HD12	2.18	0.58
1:C:364:SER:O	1:C:367:GLU:N	2.36	0.58
1:C:464:ARG:HH11	1:C:464:ARG:CB	2.17	0.58
1:B:63:ASN:ND2	1:B:63:ASN:C	2.56	0.58
1:C:249:ARG:HG2	1:C:249:ARG:HH11	1.67	0.58
1:B:56:GLY:O	1:B:59:ALA:HB3	2.03	0.58
1:D:478:LEU:HB3	1:D:479:PRO:HD2	1.85	0.58
1:D:387:GLY:O	1:D:430:ARG:HG3	2.03	0.57
1:C:106:GLU:OE2	1:C:106:GLU:HA	2.03	0.57
1:D:230:LEU:HD11	1:D:232:VAL:HG22	1.86	0.57
1:A:244:ASN:ND2	1:A:245:GLN:NE2	2.51	0.57
1:D:270:LEU:O	1:D:271:THR:HG23	2.04	0.57
1:B:340:LEU:HD22	1:B:361:CYS:HB3	1.85	0.57
1:A:283:HIS:O	1:A:287:VAL:HG23	2.04	0.57
1:D:322:THR:HG23	1:D:325:GLN:N	2.11	0.57
1:D:124:LYS:HE3	1:D:289:GLU:OE2	2.04	0.57
1:C:242:PHE:C	1:C:244:ASN:H	2.07	0.57
1:A:384:PRO:HD3	1:A:456:GLN:HE22	1.70	0.57
1:C:230:LEU:HD11	1:C:232:VAL:CG2	2.33	0.57
1:D:404:LEU:O	1:D:419:VAL:HG21	2.03	0.57
1:D:113:VAL:HG12	1:D:229:ALA:HB3	1.86	0.57
1:B:367:GLU:O	1:B:371:LEU:HD13	2.05	0.57
1:B:419:VAL:HA	1:B:441:HIS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ARG:NH1	1:C:156:ASP:OD2	2.38	0.57
1:D:79:ARG:HG3	1:D:207:THR:HG22	1.87	0.57
1:B:61:VAL:HG12	1:B:197:ILE:HD12	1.86	0.57
1:D:264:LEU:HB3	1:D:266:VAL:HG23	1.87	0.56
1:B:132:ALA:O	1:B:135:ALA:HB3	2.05	0.56
1:B:114:ASP:HB3	1:B:227:LEU:HD13	1.87	0.56
1:B:244:ASN:ND2	1:B:245:GLN:H	2.02	0.56
1:B:115:LYS:HA	1:B:231:VAL:O	2.05	0.56
1:A:244:ASN:HD22	1:A:245:GLN:N	2.02	0.56
1:C:211:LEU:N	1:C:212:PRO:HD2	2.20	0.56
1:C:239:ALA:HB3	1:C:273:MET:O	2.06	0.56
1:D:353:ASP:OD2	1:D:354:PRO:N	2.38	0.56
1:B:139:LYS:HE3	1:B:177:LEU:HB3	1.88	0.56
1:D:211:LEU:HD21	1:D:254:THR:HG21	1.88	0.56
1:C:38:GLU:O	1:C:42:MET:HG3	2.06	0.56
1:B:168:GLN:CG	1:B:185:VAL:HG11	2.36	0.56
1:A:244:ASN:HB3	1:A:247:GLN:HB3	1.88	0.56
1:C:111:GLN:O	1:C:139:LYS:HB2	2.06	0.56
1:C:364:SER:H	1:C:367:GLU:HG2	1.71	0.56
1:C:384:PRO:O	1:C:433:ARG:HG3	2.05	0.56
1:A:459:LEU:HD13	1:A:460:VAL:N	2.21	0.56
1:C:353:ASP:O	1:C:356:LEU:N	2.38	0.56
1:C:305:LEU:HD13	1:C:309:LEU:HD12	1.87	0.56
1:B:148:LEU:HD13	1:B:199:TYR:CE1	2.41	0.56
1:B:134:ALA:HA	1:B:138:CYS:O	2.06	0.55
1:D:305:LEU:HD23	1:D:472:PRO:HG2	1.86	0.55
1:D:122:GLY:HA2	1:D:286:GLU:OE2	2.06	0.55
1:D:223:LEU:CD1	1:D:262:LEU:HD13	2.35	0.55
1:D:376:ARG:HD3	1:D:443:ASP:O	2.06	0.55
1:C:291:LEU:CD1	1:C:368:ARG:HD3	2.36	0.55
1:B:413:GLU:HB2	1:B:414:PRO:HD2	1.88	0.55
1:B:120:GLY:HA2	1:B:273:MET:SD	2.47	0.55
1:D:476:LEU:HD21	1:D:478:LEU:HD21	1.88	0.55
1:D:63:ASN:HD22	1:D:63:ASN:N	2.05	0.55
1:B:428:GLY:HA3	1:B:467:PHE:O	2.06	0.55
1:C:136:CYS:SG	1:C:329:ARG:HD2	2.46	0.55
1:D:113:VAL:O	1:D:114:ASP:HB2	2.06	0.55
1:C:117:SER:HA	1:C:233:ASP:HB3	1.88	0.55
1:C:79:ARG:HG3	1:C:207:THR:HA	1.89	0.55
1:C:134:ALA:HB2	1:C:182:CYS:HB3	1.88	0.55
1:C:416:ARG:HG2	1:C:443:ASP:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:GLY:O	1:D:286:GLU:HG3	2.07	0.55
1:C:440:VAL:HG11	1:C:447:LEU:HD11	1.88	0.55
1:A:374:ARG:HH21	1:A:374:ARG:HG2	1.72	0.55
1:B:391:LEU:HD21	1:B:393:ARG:HH11	1.72	0.55
1:A:104:TRP:O	1:A:109:ARG:NH1	2.39	0.55
1:B:79:ARG:NH1	1:B:209:ASP:OD2	2.40	0.55
1:B:230:LEU:HD22	1:B:231:VAL:N	2.22	0.54
1:D:279:ARG:HD3	1:D:426:ASP:OD1	2.06	0.54
1:A:211:LEU:N	1:A:212:PRO:HD2	2.22	0.54
1:D:356:LEU:CD2	1:D:371:LEU:HD23	2.32	0.54
1:A:205:THR:O	1:A:205:THR:HG22	2.08	0.54
1:B:408:ARG:HB2	1:B:415:LEU:HD12	1.90	0.54
1:C:393:ARG:NH1	1:C:393:ARG:HG2	2.23	0.54
1:B:271:THR:HG22	1:B:473:PHE:HA	1.90	0.54
1:C:191:LEU:C	1:C:192:VAL:HG22	2.28	0.54
1:A:63:ASN:C	1:A:63:ASN:ND2	2.61	0.54
1:A:231:VAL:HG23	1:A:313:LEU:CD2	2.37	0.54
1:C:205:THR:O	1:C:206:ALA:HB3	2.07	0.54
1:D:424:LEU:HD12	1:D:436:PRO:C	2.28	0.54
1:B:219:LEU:O	1:B:223:LEU:HB2	2.08	0.54
1:C:155:LEU:O	1:C:159:GLU:HG2	2.08	0.54
1:C:284:ALA:O	1:C:288:GLU:HG3	2.07	0.54
1:C:214:ILE:HG23	1:C:218:ILE:HD12	1.90	0.54
1:C:205:THR:HG22	1:C:207:THR:HG23	1.90	0.53
1:D:108:TRP:O	1:D:112:LEU:HG	2.08	0.53
1:D:163:GLY:HA3	1:D:352:VAL:HA	1.91	0.53
1:A:285:LEU:HD21	1:A:441:HIS:HD2	1.73	0.53
1:B:244:ASN:ND2	1:B:245:GLN:N	2.56	0.53
1:C:244:ASN:HB3	1:C:247:GLN:HB3	1.89	0.53
1:D:271:THR:HG22	1:D:473:PHE:HA	1.90	0.53
1:C:312:ALA:HB2	1:C:323:GLN:OE1	2.08	0.53
1:B:408:ARG:CB	1:B:415:LEU:CD1	2.86	0.53
1:D:76:MET:CE	1:D:79:ARG:HB3	2.37	0.53
1:D:75:LEU:HD13	1:D:202:ARG:HG3	1.90	0.53
1:B:32:GLU:HG3	1:B:32:GLU:O	2.08	0.53
1:C:386:ASP:C	1:C:386:ASP:OD1	2.45	0.53
1:C:442:ARG:HG2	1:C:447:LEU:HD21	1.90	0.53
1:D:95:LEU:HD13	1:D:195:ASP:HB2	1.89	0.53
1:C:364:SER:H	1:C:367:GLU:CG	2.22	0.53
1:B:223:LEU:HD11	1:B:262:LEU:HD13	1.90	0.53
1:D:249:ARG:O	1:D:252:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:H	1:A:350:GLN:HE22	1.57	0.53
1:D:57:PHE:CZ	1:D:74:MET:HG2	2.44	0.53
1:C:148:LEU:HD13	1:C:199:TYR:CE1	2.44	0.53
1:C:230:LEU:C	1:C:230:LEU:HD13	2.28	0.53
1:B:239:ALA:HB3	1:B:273:MET:O	2.09	0.53
1:C:160:SER:CA	1:C:417:LEU:HD13	2.38	0.53
1:B:229:ALA:HB1	1:B:316:LEU:HB3	1.89	0.53
1:A:331:ALA:O	1:A:334:LEU:HB2	2.08	0.53
1:A:322:THR:HG23	1:A:325:GLN:H	1.73	0.53
1:D:76:MET:HE3	1:D:79:ARG:CB	2.39	0.53
1:B:143:ILE:HA	1:B:185:VAL:O	2.07	0.53
1:D:121:VAL:HG23	1:D:239:ALA:HB1	1.89	0.53
1:C:388:THR:HA	1:C:430:ARG:HB3	1.91	0.53
1:C:431:LEU:HD12	1:C:435:THR:HB	1.91	0.53
1:D:114:ASP:OD2	1:D:115:LYS:N	2.42	0.53
1:C:170:PRO:HA	1:C:173:MET:CE	2.34	0.52
1:D:141:PRO:HA	1:D:183:CYS:HG	1.73	0.52
1:C:386:ASP:OD1	1:C:387:GLY:N	2.43	0.52
1:B:249:ARG:HG2	1:B:270:LEU:HD11	1.91	0.52
1:A:92:THR:HG23	1:A:93:GLN:H	1.75	0.52
1:C:134:ALA:HA	1:C:138:CYS:O	2.09	0.52
1:D:130:ALA:CB	1:D:131:PRO:HD3	2.31	0.52
1:C:274:ASP:O	1:C:394:ALA:CB	2.55	0.52
1:B:278:GLY:HA2	1:B:299:PRO:CB	2.40	0.52
1:A:384:PRO:HD3	1:A:456:GLN:NE2	2.24	0.52
1:B:356:LEU:HD12	1:B:360:LEU:HD12	1.90	0.52
1:C:393:ARG:O	1:C:396:PRO:HD2	2.10	0.52
1:B:377:GLU:HB3	1:B:442:ARG:NH2	2.22	0.52
1:D:202:ARG:O	1:D:208:VAL:HG23	2.10	0.52
1:C:156:ASP:HA	1:C:159:GLU:HG3	1.90	0.52
1:D:333:ALA:HA	1:D:338:SER:HB2	1.90	0.52
1:D:356:LEU:HD13	1:D:356:LEU:C	2.30	0.52
1:C:36:LEU:HD11	1:C:66:ALA:HB2	1.92	0.52
1:C:76:MET:CE	1:C:80:LEU:HG	2.39	0.52
1:B:291:LEU:O	1:B:295:ASP:HB2	2.10	0.52
1:C:415:LEU:HD12	1:C:415:LEU:N	2.25	0.52
1:A:191:LEU:N	1:A:191:LEU:HD12	2.24	0.52
1:C:229:ALA:CB	1:C:316:LEU:HD12	2.32	0.52
1:B:402:HIS:NE2	1:B:409:SER:CB	2.69	0.52
1:D:380:GLU:HG2	1:D:439:ARG:HD3	1.91	0.52
1:D:205:THR:O	1:D:206:ALA:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLY:CA	1:C:155:LEU:HD12	2.40	0.52
1:A:168:GLN:HG2	1:A:185:VAL:HG11	1.91	0.52
1:D:277:LEU:CD2	1:D:301:ASP:HB3	2.39	0.52
1:D:387:GLY:O	1:D:431:LEU:HD23	2.09	0.52
1:D:245:GLN:NE2	1:D:245:GLN:N	2.43	0.52
1:C:76:MET:HE3	1:C:79:ARG:HB3	1.91	0.52
1:C:277:LEU:HD12	1:C:302:LEU:HD23	1.92	0.52
1:D:289:GLU:HG2	1:D:302:LEU:HD11	1.92	0.51
1:C:113:VAL:HA	1:C:229:ALA:O	2.09	0.51
1:D:388:THR:N	1:D:430:ARG:NH1	2.58	0.51
1:C:329:ARG:O	1:C:332:ALA:HB3	2.10	0.51
1:D:176:LEU:HD21	1:D:350:GLN:HE21	1.76	0.51
1:A:426:ASP:N	1:A:429:GLN:HE21	1.91	0.51
1:B:431:LEU:HD11	1:B:437:TRP:HB3	1.91	0.51
1:C:143:ILE:HG12	1:C:185:VAL:HG23	1.91	0.51
1:C:205:THR:O	1:C:205:THR:CG2	2.59	0.51
1:A:303:ARG:NH1	1:A:335:ASP:OD1	2.43	0.51
1:D:83:MET:HE3	1:D:87:GLU:HB3	1.91	0.51
1:B:83:MET:HB3	1:B:87:GLU:HB2	1.92	0.51
1:C:77:ALA:O	1:C:81:ARG:HB2	2.10	0.51
1:C:256:VAL:HG23	1:C:266:VAL:HG23	1.92	0.51
1:B:205:THR:O	1:B:205:THR:CG2	2.57	0.51
1:D:389:VAL:HG23	1:D:431:LEU:HD22	1.90	0.51
1:B:232:VAL:HG11	1:B:255:LEU:HD13	1.92	0.51
1:C:215:THR:HG22	1:C:219:LEU:HD12	1.92	0.51
1:C:191:LEU:O	1:C:192:VAL:HG23	2.11	0.51
1:B:285:LEU:CD2	1:B:369:ARG:HH21	2.21	0.51
1:C:238:GLY:O	1:C:395:LEU:HD22	2.11	0.51
1:D:83:MET:CE	1:D:87:GLU:HB3	2.41	0.51
1:B:172:GLN:O	1:B:175:VAL:HG12	2.10	0.51
1:D:95:LEU:HD21	1:D:198:LEU:HD12	1.93	0.51
1:D:340:LEU:HD22	1:D:340:LEU:O	2.11	0.51
1:A:183:CYS:HB2	1:A:350:GLN:NE2	2.26	0.51
1:D:387:GLY:C	1:D:430:ARG:HG3	2.32	0.51
1:B:253:LYS:O	1:B:256:VAL:HG23	2.11	0.50
1:B:133:LEU:HD11	1:B:313:LEU:HD12	1.92	0.50
1:D:414:PRO:O	1:D:415:LEU:CD1	2.59	0.50
1:C:205:THR:O	1:C:205:THR:HG22	2.11	0.50
1:D:251:LEU:C	1:D:251:LEU:HD13	2.32	0.50
1:D:153:GLY:O	1:D:157:LYS:HG2	2.11	0.50
1:C:385:ALA:O	1:C:386:ASP:C	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:VAL:CG1	1:D:224:VAL:HG21	2.40	0.50
1:C:85:LEU:HD22	1:C:85:LEU:N	2.25	0.50
1:A:148:LEU:HD13	1:A:199:TYR:CE1	2.47	0.50
1:C:74:MET:O	1:C:78:ILE:HG13	2.10	0.50
1:A:117:SER:HA	1:A:233:ASP:HB3	1.93	0.50
1:A:459:LEU:HD11	1:A:461:LEU:HG	1.93	0.50
1:B:84:ASP:OD2	1:B:87:GLU:HG3	2.10	0.50
1:B:205:THR:HG22	1:B:207:THR:HG23	1.93	0.50
1:B:304:ASP:OD1	1:B:472:PRO:HD2	2.12	0.50
1:B:131:PRO:HB2	1:B:294:MET:HE1	1.93	0.50
1:A:364:SER:HB3	1:C:97:GLN:O	2.10	0.50
1:C:276:PRO:HD3	1:C:394:ALA:HB2	1.92	0.50
1:C:156:ASP:OD2	1:C:408:ARG:NH2	2.44	0.50
1:B:245:GLN:O	1:B:249:ARG:HG3	2.11	0.50
1:B:252:ALA:O	1:B:256:VAL:HG22	2.11	0.50
1:B:378:GLN:HE21	1:B:439:ARG:HD3	1.73	0.50
1:D:413:GLU:O	1:D:414:PRO:O	2.30	0.50
1:C:364:SER:N	1:C:367:GLU:HG2	2.26	0.50
1:B:166:VAL:HG23	1:B:167:ILE:CD1	2.40	0.50
1:B:124:LYS:H	1:B:124:LYS:HD2	1.77	0.50
1:B:195:ASP:OD1	1:B:221:LYS:HE3	2.11	0.50
1:D:120:GLY:HA3	1:D:273:MET:CE	2.41	0.50
1:A:246:GLU:C	1:A:248:ALA:H	2.14	0.50
1:D:369:ARG:O	1:D:374:ARG:HD3	2.12	0.50
1:A:215:THR:HG22	1:A:219:LEU:HD12	1.94	0.50
1:B:50:SER:C	1:B:52:ALA:N	2.65	0.50
1:C:381:LEU:O	1:C:382:LEU:O	2.30	0.49
1:A:316:LEU:C	1:A:318:GLY:H	2.16	0.49
1:B:391:LEU:HD11	1:B:393:ARG:HH11	1.76	0.49
1:D:211:LEU:C	1:D:211:LEU:HD23	2.32	0.49
1:C:113:VAL:O	1:C:114:ASP:HB2	2.12	0.49
1:D:36:LEU:HB3	1:D:37:PRO:HD3	1.92	0.49
1:D:43:LYS:HG3	1:D:74:MET:CE	2.42	0.49
1:B:133:LEU:O	1:B:138:CYS:HB2	2.12	0.49
1:A:116:HIS:CD2	1:A:218:ILE:HG23	2.48	0.49
1:D:367:GLU:O	1:D:370:GLN:HB2	2.12	0.49
1:C:384:PRO:CD	1:C:459:LEU:HD13	2.42	0.49
1:D:431:LEU:HD23	1:D:431:LEU:N	2.26	0.49
1:B:340:LEU:CD2	1:B:361:CYS:HB3	2.43	0.49
1:B:127:LEU:HD22	1:B:158:LEU:HD21	1.93	0.49
1:D:291:LEU:O	1:D:295:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:HD13	1:C:199:TYR:CZ	2.48	0.49
1:C:125:VAL:HG13	1:C:306:VAL:CG2	2.42	0.49
1:C:393:ARG:CG	1:C:396:PRO:HG2	2.40	0.49
1:B:146:ARG:C	1:B:153:GLY:HA3	2.33	0.49
1:B:118:THR:HG22	1:B:218:ILE:HD11	1.94	0.49
1:D:363:GLY:O	1:D:364:SER:O	2.30	0.49
1:B:139:LYS:HE3	1:B:177:LEU:O	2.13	0.49
1:A:173:MET:HA	1:A:176:LEU:HD12	1.94	0.49
1:B:442:ARG:NH2	1:B:442:ARG:HG3	2.27	0.49
1:B:231:VAL:HG23	1:B:313:LEU:HD23	1.93	0.49
1:D:388:THR:HA	1:D:430:ARG:HA	1.94	0.49
1:D:321:GLY:H	1:D:325:GLN:NE2	2.11	0.49
1:D:124:LYS:NZ	1:D:280:CYS:O	2.44	0.49
1:C:36:LEU:HB2	1:C:37:PRO:HD3	1.94	0.49
1:C:379:GLU:HG2	1:C:442:ARG:HD3	1.94	0.49
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.76	0.49
1:C:291:LEU:HD13	1:C:368:ARG:HD3	1.95	0.49
1:B:51:GLU:HA	1:B:90:VAL:HG11	1.95	0.49
1:C:386:ASP:H	1:C:433:ARG:HB2	1.76	0.49
1:C:211:LEU:HD21	1:C:251:LEU:HA	1.93	0.49
1:B:290:ALA:O	1:B:294:MET:HG3	2.13	0.49
1:D:236:PHE:CE2	1:D:474:ALA:HB2	2.47	0.49
1:C:292:LEU:HD11	1:C:365:PRO:CG	2.43	0.49
1:D:180:ALA:O	1:D:342:ARG:HG3	2.13	0.49
1:C:275:LYS:HD2	1:C:427:VAL:HG21	1.94	0.49
1:D:388:THR:OG1	1:D:430:ARG:NH1	2.46	0.49
1:D:365:PRO:O	1:D:367:GLU:N	2.46	0.49
1:A:190:GLN:HB2	1:A:191:LEU:HD12	1.95	0.49
1:D:376:ARG:NH1	1:D:377:GLU:HB2	2.28	0.49
1:D:365:PRO:O	1:D:368:ARG:HB2	2.12	0.48
1:B:379:GLU:HG2	1:B:442:ARG:HH11	1.78	0.48
1:C:112:LEU:HD23	1:C:139:LYS:O	2.13	0.48
1:C:234:VAL:HG11	1:C:248:ALA:O	2.14	0.48
1:C:192:VAL:N	1:C:193:PRO:HD3	2.28	0.48
1:B:253:LYS:HA	1:B:256:VAL:CG2	2.43	0.48
1:D:205:THR:HG22	1:D:207:THR:HG23	1.94	0.48
1:A:249:ARG:HG3	1:A:270:LEU:HD11	1.94	0.48
1:C:352:VAL:HG12	1:C:353:ASP:N	2.28	0.48
1:C:437:TRP:CE2	1:C:459:LEU:HD12	2.48	0.48
1:C:133:LEU:CD1	1:C:313:LEU:HD12	2.42	0.48
1:A:459:LEU:C	1:A:459:LEU:HD13	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:LEU:O	1:C:382:LEU:C	2.52	0.48
1:A:191:LEU:C	1:A:193:PRO:HD3	2.33	0.48
1:D:294:MET:HE2	1:D:343:PHE:HB2	1.95	0.48
1:B:114:ASP:HB3	1:B:227:LEU:CD1	2.43	0.48
1:B:231:VAL:HG23	1:B:313:LEU:CD2	2.43	0.48
1:D:381:LEU:HD23	1:D:438:LEU:HD23	1.96	0.48
1:A:370:GLN:HA	1:A:374:ARG:CZ	2.43	0.48
1:D:281:VAL:HA	1:D:286:GLU:OE2	2.14	0.48
1:B:101:GLN:HE22	1:B:224:VAL:HG23	1.78	0.48
1:D:367:GLU:HA	1:D:367:GLU:OE2	2.13	0.48
1:D:172:GLN:O	1:D:176:LEU:HD13	2.13	0.48
1:D:161:ILE:HD12	1:D:360:LEU:HD21	1.95	0.48
1:C:188:SER:C	1:C:190:GLN:H	2.17	0.48
1:D:36:LEU:HD11	1:D:57:PHE:CD1	2.43	0.48
1:A:246:GLU:C	1:A:248:ALA:N	2.66	0.48
1:A:54:ILE:O	1:A:58:VAL:HG23	2.13	0.48
1:C:265:ARG:HD2	1:C:316:LEU:CD1	2.43	0.48
1:A:118:THR:HG23	1:A:233:ASP:O	2.14	0.48
1:A:432:ARG:O	1:A:435:THR:HG23	2.13	0.48
1:C:188:SER:O	1:C:193:PRO:HG3	2.13	0.48
1:A:104:TRP:N	1:A:109:ARG:HH12	2.06	0.48
1:D:63:ASN:ND2	1:D:65:SER:H	2.12	0.48
1:A:122:GLY:O	1:A:124:LYS:NZ	2.41	0.48
1:B:323:GLN:O	1:B:327:ALA:N	2.37	0.48
1:C:295:ASP:O	1:C:296:GLY:C	2.51	0.48
1:A:158:LEU:HD13	1:A:164:PHE:CZ	2.49	0.48
1:C:128:VAL:O	1:C:131:PRO:HD2	2.14	0.48
1:D:158:LEU:HD13	1:D:164:PHE:CZ	2.49	0.47
1:B:174:GLN:HG3	1:B:175:VAL:N	2.28	0.47
1:D:36:LEU:HD23	1:D:70:GLN:CD	2.35	0.47
1:A:168:GLN:HG2	1:A:185:VAL:CG1	2.44	0.47
1:D:284:ALA:O	1:D:288:GLU:HG3	2.14	0.47
1:C:235:LYS:HE3	1:C:273:MET:CG	2.43	0.47
1:D:356:LEU:HD21	1:D:371:LEU:HB3	1.95	0.47
1:C:230:LEU:HD11	1:C:232:VAL:HG23	1.96	0.47
1:D:244:ASN:HB3	1:D:247:GLN:CB	2.42	0.47
1:D:294:MET:CE	1:D:343:PHE:HB2	2.44	0.47
1:A:89:SER:O	1:A:92:THR:HG23	2.13	0.47
1:D:60:ALA:HB1	1:D:66:ALA:HB2	1.96	0.47
1:B:265:ARG:HD2	1:B:316:LEU:CD1	2.44	0.47
1:A:241:VAL:O	1:A:243:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:HB3	1:A:168:GLN:NE2	2.26	0.47
1:A:244:ASN:HD21	1:A:245:GLN:NE2	2.11	0.47
1:D:391:LEU:HD23	1:D:391:LEU:C	2.34	0.47
1:A:382:LEU:HD22	1:A:434:GLY:O	2.14	0.47
1:D:402:HIS:ND1	1:D:407:GLY:HA3	2.30	0.47
1:A:219:LEU:O	1:A:223:LEU:HG	2.14	0.47
1:B:175:VAL:CG1	1:B:176:LEU:N	2.77	0.47
1:A:252:ALA:O	1:A:256:VAL:HG23	2.15	0.47
1:A:106:GLU:O	1:A:109:ARG:HB2	2.14	0.47
1:B:379:GLU:HG2	1:B:442:ARG:NH1	2.29	0.47
1:C:438:LEU:HG	1:C:439:ARG:N	2.29	0.47
1:D:192:VAL:HG21	1:D:221:LYS:HG2	1.96	0.47
1:B:204:VAL:HG12	1:B:409:SER:HA	1.95	0.47
1:A:390:GLU:O	1:A:427:VAL:HG13	2.14	0.47
1:D:285:LEU:HD11	1:D:441:HIS:HD2	1.80	0.47
1:C:463:ASP:N	1:C:463:ASP:OD2	2.46	0.47
1:A:445:PRO:O	1:A:446:ALA:CB	2.59	0.47
1:D:92:THR:HG22	1:D:216:ALA:HA	1.96	0.47
1:C:348:ALA:HB1	1:C:354:PRO:HG3	1.96	0.47
1:B:34:LYS:HE3	1:B:42:MET:CE	2.44	0.47
1:A:367:GLU:O	1:A:371:LEU:HD12	2.15	0.47
1:C:119:GLY:O	1:C:235:LYS:HG3	2.15	0.47
1:C:143:ILE:HA	1:C:185:VAL:O	2.15	0.47
1:D:148:LEU:HD13	1:D:199:TYR:CZ	2.50	0.47
1:C:192:VAL:HG13	1:C:224:VAL:HG21	1.96	0.47
1:D:76:MET:CE	1:D:80:LEU:HG	2.45	0.47
1:C:299:PRO:HA	1:C:300:PRO:HD3	1.79	0.47
1:C:307:THR:HA	1:C:330:VAL:HG11	1.97	0.47
1:B:460:VAL:O	1:B:461:LEU:HD23	2.14	0.47
1:C:384:PRO:HG2	1:C:385:ALA:H	1.80	0.47
1:C:424:LEU:O	1:C:425:VAL:HG13	2.15	0.47
1:C:191:LEU:C	1:C:192:VAL:CG2	2.83	0.47
1:B:244:ASN:HD22	1:B:245:GLN:H	1.62	0.47
1:A:391:LEU:HD23	1:A:460:VAL:CG2	2.44	0.47
1:C:247:GLN:C	1:C:249:ARG:H	2.18	0.47
1:B:148:LEU:HD21	1:B:202:ARG:CZ	2.45	0.47
1:C:319:HIS:CD2	1:C:319:HIS:N	2.83	0.47
1:C:367:GLU:O	1:C:371:LEU:HD13	2.15	0.47
1:B:333:ALA:HB1	1:B:339:ALA:HB2	1.96	0.47
1:C:453:ARG:NH1	1:C:453:ARG:CB	2.74	0.46
1:D:276:PRO:CG	1:D:397:LEU:HD23	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:HD21	1:A:310:GLY:HA2	1.98	0.46
1:C:478:LEU:CG	1:C:479:PRO:HD2	2.45	0.46
1:C:305:LEU:HD13	1:C:309:LEU:CD1	2.45	0.46
1:B:249:ARG:O	1:B:252:ALA:HB3	2.15	0.46
1:C:390:GLU:HB2	1:C:460:VAL:O	2.15	0.46
1:D:383:ALA:HB2	1:D:431:LEU:HD12	1.97	0.46
1:D:430:ARG:HH11	1:D:430:ARG:HG3	1.81	0.46
1:C:125:VAL:HG13	1:C:306:VAL:HG22	1.96	0.46
1:A:232:VAL:HG11	1:A:255:LEU:HD12	1.97	0.46
1:B:39:LEU:HD22	1:B:53:ASP:HB3	1.96	0.46
1:C:473:PHE:HZ	1:C:476:LEU:HB2	1.80	0.46
1:D:296:GLY:O	1:D:297:ALA:HB2	2.15	0.46
1:D:416:ARG:HH11	1:D:443:ASP:CG	2.14	0.46
1:D:111:GLN:O	1:D:139:LYS:N	2.47	0.46
1:A:80:LEU:O	1:A:81:ARG:HD2	2.15	0.46
1:C:236:PHE:O	1:C:236:PHE:CD1	2.69	0.46
1:D:38:GLU:O	1:D:42:MET:HG3	2.15	0.46
1:A:205:THR:CG2	1:A:207:THR:OG1	2.63	0.46
1:D:60:ALA:CB	1:D:66:ALA:HB2	2.46	0.46
1:C:388:THR:HA	1:C:430:ARG:HB2	1.96	0.46
1:C:214:ILE:HA	1:C:214:ILE:HD13	1.86	0.46
1:B:347:LEU:HB3	1:B:352:VAL:HG21	1.97	0.46
1:D:455:LEU:O	1:D:458:ALA:HB3	2.15	0.46
1:D:345:ARG:O	1:D:349:ALA:HB2	2.16	0.46
1:C:347:LEU:O	1:C:352:VAL:HG23	2.16	0.46
1:D:115:LYS:C	1:D:115:LYS:HD2	2.36	0.46
1:C:437:TRP:NE1	1:C:459:LEU:HD12	2.30	0.46
1:A:106:GLU:HA	1:A:109:ARG:HD3	1.98	0.46
1:D:233:ASP:OD1	1:D:271:THR:OG1	2.33	0.46
1:A:292:LEU:HD22	1:A:298:GLY:CA	2.45	0.46
1:C:43:LYS:HE3	1:C:43:LYS:HA	1.98	0.46
1:B:246:GLU:HA	1:B:249:ARG:HD3	1.97	0.46
1:C:242:PHE:O	1:C:244:ASN:N	2.48	0.46
1:B:134:ALA:HB2	1:B:182:CYS:HB3	1.98	0.46
1:D:215:THR:HG23	1:D:255:LEU:HD23	1.97	0.46
1:A:146:ARG:NH1	1:A:156:ASP:OD2	2.44	0.46
1:C:83:MET:HB2	1:C:87:GLU:OE2	2.16	0.46
1:C:419:VAL:HG12	1:C:420:GLY:N	2.31	0.46
1:D:353:ASP:C	1:D:353:ASP:OD2	2.55	0.45
1:D:244:ASN:C	1:D:244:ASN:HD22	2.19	0.45
1:D:75:LEU:HD13	1:D:202:ARG:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASN:C	1:A:244:ASN:HD22	2.19	0.45
1:B:408:ARG:CB	1:B:415:LEU:HD12	2.45	0.45
1:B:89:SER:HA	1:B:92:THR:HG22	1.97	0.45
1:C:143:ILE:HG12	1:C:185:VAL:CG2	2.45	0.45
1:B:50:SER:C	1:B:52:ALA:H	2.19	0.45
1:C:265:ARG:HH11	1:C:265:ARG:CB	2.28	0.45
1:D:422:GLU:O	1:D:438:LEU:HD12	2.16	0.45
1:C:416:ARG:HB2	1:C:419:VAL:HG23	1.97	0.45
1:B:202:ARG:HA	1:B:207:THR:OG1	2.15	0.45
1:C:135:ALA:HA	1:C:342:ARG:HH11	1.78	0.45
1:D:307:THR:HA	1:D:330:VAL:HG11	1.97	0.45
1:A:153:GLY:O	1:A:157:LYS:HG3	2.17	0.45
1:B:146:ARG:HH11	1:B:146:ARG:HG2	1.81	0.45
1:A:211:LEU:HD13	1:A:211:LEU:C	2.37	0.45
1:B:131:PRO:HB2	1:B:294:MET:CE	2.46	0.45
1:D:425:VAL:HG11	1:D:431:LEU:HD13	1.98	0.45
1:B:352:VAL:HG12	1:B:356:LEU:HB3	1.98	0.45
1:C:431:LEU:HD21	1:C:461:LEU:HD21	1.97	0.45
1:C:100:GLN:O	1:C:101:GLN:NE2	2.50	0.45
1:C:36:LEU:N	1:C:37:PRO:CD	2.79	0.45
1:A:393:ARG:HB3	1:A:396:PRO:HD2	1.98	0.45
1:C:333:ALA:HA	1:C:336:ASP:OD2	2.17	0.45
1:C:344:GLU:HB2	1:C:361:CYS:SG	2.56	0.45
1:C:242:PHE:C	1:C:244:ASN:N	2.70	0.45
1:B:378:GLN:HB2	1:B:440:VAL:O	2.17	0.45
1:C:279:ARG:HG2	1:C:279:ARG:NH2	2.31	0.45
1:D:211:LEU:HD23	1:D:212:PRO:N	2.32	0.45
1:A:34:LYS:HD2	1:A:39:LEU:CD2	2.47	0.45
1:A:135:ALA:HB1	1:A:338:SER:HB3	1.98	0.45
1:A:373:PRO:O	1:A:418:GLY:HA2	2.17	0.45
1:A:98:SER:OG	1:A:193:PRO:HD2	2.17	0.45
1:A:205:THR:O	1:A:206:ALA:HB3	2.16	0.45
1:B:256:VAL:HA	1:B:266:VAL:HB	1.98	0.45
1:B:285:LEU:HD21	1:B:369:ARG:HH22	1.76	0.45
1:C:276:PRO:CD	1:C:394:ALA:HB2	2.47	0.45
1:A:244:ASN:ND2	1:A:244:ASN:C	2.70	0.45
1:A:101:GLN:H	1:A:101:GLN:NE2	2.14	0.45
1:B:432:ARG:O	1:B:433:ARG:C	2.54	0.45
1:D:83:MET:HB2	1:D:87:GLU:HB2	1.99	0.45
1:C:342:ARG:HA	1:C:342:ARG:HD2	1.84	0.45
1:A:48:ARG:NH1	1:A:84:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:SER:OG	1:B:52:ALA:HB3	2.16	0.45
1:A:382:LEU:CD2	1:A:436:PRO:HG3	2.47	0.45
1:D:416:ARG:HB2	1:D:419:VAL:CG2	2.46	0.45
1:B:115:LYS:HG2	1:B:129:LEU:CD1	2.46	0.45
1:C:288:GLU:CG	1:C:372:LEU:HD12	2.47	0.45
1:A:54:ILE:HD12	1:A:90:VAL:HB	1.99	0.45
1:C:195:ASP:OD1	1:C:221:LYS:HE2	2.16	0.45
1:C:451:GLN:O	1:C:455:LEU:N	2.47	0.45
1:A:117:SER:OG	1:A:118:THR:N	2.50	0.45
1:B:249:ARG:CG	1:B:270:LEU:HD11	2.47	0.45
1:D:375:ALA:HB3	1:D:441:HIS:HB3	1.97	0.44
1:D:260:ALA:HA	1:D:264:LEU:O	2.17	0.44
1:D:117:SER:HA	1:D:233:ASP:HB3	1.99	0.44
1:A:231:VAL:HG23	1:A:313:LEU:HD23	1.97	0.44
1:B:113:VAL:HB	1:B:313:LEU:HD22	1.99	0.44
1:B:127:LEU:CD2	1:B:158:LEU:HD21	2.47	0.44
1:D:176:LEU:HD23	1:D:183:CYS:HB2	1.99	0.44
1:C:164:PHE:CE2	1:C:347:LEU:HD23	2.53	0.44
1:C:85:LEU:CD2	1:C:85:LEU:N	2.79	0.44
1:B:86:GLU:O	1:B:90:VAL:HG23	2.17	0.44
1:A:299:PRO:HA	1:A:300:PRO:HD3	1.86	0.44
1:C:102:LEU:HD13	1:C:104:TRP:CZ2	2.53	0.44
1:B:167:ILE:N	1:B:167:ILE:HD12	2.32	0.44
1:D:120:GLY:HA3	1:D:273:MET:HE2	1.98	0.44
1:C:235:LYS:HE3	1:C:273:MET:HG3	1.99	0.44
1:A:230:LEU:HD12	1:A:266:VAL:HG22	1.99	0.44
1:B:390:GLU:O	1:B:391:LEU:HB3	2.17	0.44
1:B:113:VAL:O	1:B:114:ASP:HB2	2.16	0.44
1:A:432:ARG:HD3	1:A:432:ARG:N	2.31	0.44
1:A:202:ARG:CD	1:A:213:LEU:HD13	2.48	0.44
1:C:36:LEU:H	1:C:37:PRO:HD2	1.83	0.44
1:B:273:MET:HE1	1:B:276:PRO:HA	2.00	0.44
1:B:195:ASP:O	1:B:199:TYR:HB2	2.18	0.44
1:A:210:SER:C	1:A:212:PRO:HD2	2.38	0.44
1:A:48:ARG:HH12	1:A:87:GLU:HG3	1.79	0.44
1:D:251:LEU:HD13	1:D:251:LEU:O	2.17	0.44
1:C:175:VAL:O	1:C:179:GLN:N	2.49	0.44
1:D:291:LEU:O	1:D:295:ASP:N	2.50	0.44
1:C:376:ARG:HG3	1:C:443:ASP:OD2	2.16	0.44
1:C:379:GLU:OE1	1:C:442:ARG:HD3	2.18	0.44
1:C:279:ARG:HB3	1:C:423:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ARG:HD3	1:B:410:ARG:HA	1.64	0.44
1:C:215:THR:HG23	1:C:255:LEU:HD23	1.99	0.44
1:A:476:LEU:O	1:A:478:LEU:HD12	2.17	0.44
1:C:160:SER:HA	1:C:417:LEU:CD1	2.47	0.44
1:C:46:GLY:HA2	1:C:81:ARG:HG3	1.98	0.44
1:A:279:ARG:H	1:A:289:GLU:CD	2.20	0.44
1:B:75:LEU:HA	1:B:75:LEU:HD23	1.78	0.44
1:D:245:GLN:CD	1:D:245:GLN:N	2.62	0.44
1:A:131:PRO:HG2	1:A:343:PHE:HD1	1.82	0.44
1:D:106:GLU:CA	1:D:109:ARG:HH11	2.29	0.44
1:B:89:SER:C	1:B:92:THR:HG22	2.39	0.44
1:A:245:GLN:H	1:A:245:GLN:CD	2.21	0.44
1:C:277:LEU:CD1	1:C:302:LEU:HD23	2.47	0.44
1:D:148:LEU:HD13	1:D:199:TYR:CE1	2.52	0.44
1:B:246:GLU:O	1:B:250:GLU:HG2	2.18	0.44
1:C:340:LEU:HD11	1:C:361:CYS:HB3	1.99	0.44
1:D:416:ARG:HD3	1:D:443:ASP:OD1	2.17	0.44
1:D:264:LEU:HB3	1:D:266:VAL:CG2	2.47	0.44
1:B:128:VAL:HA	1:B:294:MET:HE3	2.00	0.44
1:C:291:LEU:HD12	1:C:368:ARG:HD3	2.00	0.44
1:B:283:HIS:HE2	1:B:415:LEU:CD2	2.27	0.43
1:C:459:LEU:CD2	1:C:461:LEU:HG	2.42	0.43
1:C:34:LYS:O	1:C:35:GLN:O	2.36	0.43
1:A:391:LEU:CD2	1:A:460:VAL:HG21	2.47	0.43
1:B:278:GLY:HA2	1:B:299:PRO:HB2	2.00	0.43
1:A:148:LEU:HD13	1:A:199:TYR:CZ	2.52	0.43
1:D:146:ARG:HG2	1:D:155:LEU:HB2	1.99	0.43
1:A:265:ARG:HG2	1:A:316:LEU:HD11	1.99	0.43
1:C:364:SER:N	1:C:367:GLU:CG	2.81	0.43
1:D:157:LYS:HE3	1:D:286:GLU:CD	2.38	0.43
1:C:211:LEU:HB3	1:C:212:PRO:HD3	2.01	0.43
1:B:279:ARG:HH21	1:B:426:ASP:CG	2.21	0.43
1:A:202:ARG:HD3	1:A:213:LEU:HD13	1.99	0.43
1:A:118:THR:HG1	1:A:119:GLY:H	1.56	0.43
1:B:379:GLU:CD	1:B:442:ARG:HE	2.21	0.43
1:D:211:LEU:N	1:D:212:PRO:HD2	2.33	0.43
1:A:367:GLU:C	1:A:371:LEU:HD12	2.38	0.43
1:D:79:ARG:HG3	1:D:207:THR:CA	2.41	0.43
1:C:401:LEU:HD13	1:C:404:LEU:CD1	2.44	0.43
1:A:389:VAL:HG12	1:A:427:VAL:HA	2.00	0.43
1:D:63:ASN:H	1:D:63:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ARG:CG	1:C:279:ARG:HH21	2.31	0.43
1:B:133:LEU:CD1	1:B:313:LEU:HD12	2.48	0.43
1:B:428:GLY:HA2	1:B:467:PHE:CD2	2.54	0.43
1:B:277:LEU:HD11	1:B:305:LEU:HD12	2.00	0.43
1:D:176:LEU:HD23	1:D:183:CYS:CB	2.48	0.43
1:C:232:VAL:HG11	1:C:255:LEU:HD13	2.01	0.43
1:B:381:LEU:CD1	1:B:438:LEU:HD23	2.35	0.43
1:B:383:ALA:CB	1:B:431:LEU:HD22	2.48	0.43
1:D:201:ALA:O	1:D:202:ARG:C	2.57	0.43
1:B:141:PRO:O	1:B:225:GLU:OE1	2.36	0.43
1:A:321:GLY:HA3	1:A:325:GLN:OE1	2.18	0.43
1:C:265:ARG:HH11	1:C:265:ARG:CG	2.31	0.43
1:A:79:ARG:C	1:A:79:ARG:HD3	2.37	0.43
1:C:48:ARG:CD	1:C:84:ASP:OD2	2.57	0.43
1:D:76:MET:HE2	1:D:80:LEU:HG	1.99	0.43
1:B:48:ARG:NH1	1:B:87:GLU:HG2	2.34	0.43
1:B:79:ARG:HG3	1:B:207:THR:HA	1.99	0.43
1:A:269:ALA:HB2	1:A:476:LEU:CD1	2.45	0.43
1:B:129:LEU:HD22	1:B:133:LEU:CD1	2.48	0.43
1:B:192:VAL:N	1:B:193:PRO:HD3	2.34	0.43
1:D:387:GLY:C	1:D:430:ARG:HH11	2.22	0.43
1:C:237:GLY:O	1:C:240:ALA:N	2.46	0.43
1:D:424:LEU:CD1	1:D:436:PRO:HB2	2.48	0.43
1:C:346:MET:HG2	1:C:346:MET:O	2.18	0.43
1:A:308:THR:HG21	1:A:473:PHE:CD2	2.54	0.43
1:B:222:LYS:HA	1:B:222:LYS:HD3	1.84	0.43
1:D:456:GLN:NE2	1:D:456:GLN:CA	2.75	0.43
1:D:299:PRO:HD2	1:D:302:LEU:HD12	2.00	0.43
1:A:130:ALA:HB3	1:A:131:PRO:CD	2.35	0.43
1:A:391:LEU:HA	1:A:427:VAL:CG2	2.46	0.43
1:D:105:PRO:HD2	1:D:108:TRP:CE3	2.54	0.43
1:A:214:ILE:O	1:A:218:ILE:HG13	2.17	0.43
1:A:439:ARG:HD2	1:A:441:HIS:CE1	2.53	0.43
1:D:124:LYS:HG2	1:D:124:LYS:H	1.49	0.43
1:A:229:ALA:CB	1:A:316:LEU:HD12	2.38	0.43
1:C:111:GLN:HG3	1:C:319:HIS:HE1	1.83	0.43
1:A:83:MET:HB3	1:A:87:GLU:HB2	2.00	0.43
1:D:211:LEU:HB3	1:D:212:PRO:CD	2.49	0.43
1:D:115:LYS:HD2	1:D:116:HIS:N	2.33	0.43
1:B:158:LEU:C	1:B:160:SER:H	2.21	0.43
1:C:184:ILE:H	1:C:350:GLN:HE22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:CB	1:A:131:PRO:HD3	2.36	0.43
1:D:275:LYS:HG3	1:D:276:PRO:O	2.19	0.43
1:C:142:MET:O	1:C:184:ILE:HA	2.19	0.43
1:C:141:PRO:O	1:C:225:GLU:CD	2.57	0.43
1:C:397:LEU:HD22	1:C:401:LEU:HD23	2.01	0.43
1:C:164:PHE:HE2	1:C:347:LEU:HD23	1.84	0.43
1:D:442:ARG:NH2	1:D:444:GLY:O	2.47	0.43
1:C:49:LEU:HA	1:C:49:LEU:HD12	1.87	0.43
1:B:223:LEU:HA	1:B:264:LEU:HD11	2.00	0.42
1:A:176:LEU:HD22	1:A:350:GLN:HE21	1.84	0.42
1:C:462:SER:OG	1:C:463:ASP:N	2.52	0.42
1:A:268:ALA:O	1:A:477:VAL:N	2.52	0.42
1:B:382:LEU:HD22	1:B:434:GLY:O	2.19	0.42
1:B:421:ALA:HB1	1:B:438:LEU:HD11	2.01	0.42
1:A:390:GLU:CD	1:A:464:ARG:HH21	2.22	0.42
1:C:442:ARG:H	1:C:442:ARG:HG3	1.64	0.42
1:C:356:LEU:O	1:C:359:ALA:HB3	2.19	0.42
1:C:106:GLU:OE2	1:C:109:ARG:HD3	2.19	0.42
1:A:202:ARG:HE	1:A:208:VAL:HA	1.84	0.42
1:C:36:LEU:N	1:C:37:PRO:HD2	2.34	0.42
1:B:166:VAL:O	1:B:185:VAL:HB	2.20	0.42
1:B:49:LEU:HB2	1:B:54:ILE:HD13	2.01	0.42
1:D:114:ASP:HB3	1:D:227:LEU:CD1	2.49	0.42
1:D:139:LYS:HA	1:D:181:GLY:O	2.20	0.42
1:A:63:ASN:HD21	1:A:65:SER:H	1.66	0.42
1:C:111:GLN:HG3	1:C:137:GLY:O	2.20	0.42
1:D:57:PHE:CE2	1:D:74:MET:HG2	2.54	0.42
1:D:389:VAL:CG2	1:D:431:LEU:HD22	2.49	0.42
1:D:374:ARG:HG2	1:D:374:ARG:HH21	1.84	0.42
1:C:222:LYS:HA	1:C:222:LYS:HD3	1.82	0.42
1:B:108:TRP:O	1:B:112:LEU:HG	2.19	0.42
1:A:343:PHE:CZ	1:A:347:LEU:HD21	2.55	0.42
1:D:43:LYS:HG3	1:D:74:MET:HE1	2.01	0.42
1:C:79:ARG:CG	1:C:207:THR:HG22	2.49	0.42
1:D:391:LEU:HG	1:D:392:VAL:N	2.34	0.42
1:C:177:LEU:O	1:C:181:GLY:HA2	2.20	0.42
1:D:371:LEU:H	1:D:371:LEU:CD1	2.33	0.42
1:D:131:PRO:HB2	1:D:294:MET:CE	2.50	0.42
1:A:238:GLY:HA3	1:A:274:ASP:HA	2.02	0.42
1:D:468:ALA:O	1:D:469:ALA:C	2.57	0.42
1:A:202:ARG:HD2	1:A:207:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ASP:CG	1:C:87:GLU:HG3	2.41	0.42
1:B:89:SER:HA	1:B:92:THR:CG2	2.50	0.42
1:B:478:LEU:O	1:B:480:PRO:CD	2.68	0.42
1:A:292:LEU:HD22	1:A:298:GLY:HA2	2.01	0.42
1:A:132:ALA:HB1	1:A:330:VAL:HG13	2.02	0.42
1:A:62:VAL:HG21	1:A:98:SER:HB2	2.02	0.42
1:C:113:VAL:HG23	1:C:140:VAL:HG22	2.02	0.42
1:D:424:LEU:HD12	1:D:436:PRO:HB2	2.02	0.42
1:C:478:LEU:HD12	1:C:479:PRO:CD	2.42	0.41
1:D:236:PHE:HE2	1:D:474:ALA:CB	2.33	0.41
1:A:236:PHE:CD1	1:A:236:PHE:C	2.94	0.41
1:B:210:SER:HB3	1:B:213:LEU:HB2	2.01	0.41
1:C:424:LEU:HB2	1:C:437:TRP:C	2.41	0.41
1:D:130:ALA:HB3	1:D:131:PRO:CD	2.33	0.41
1:B:120:GLY:HA2	1:B:273:MET:HG2	2.03	0.41
1:C:306:VAL:HG12	1:C:307:THR:N	2.36	0.41
1:D:401:LEU:HD11	1:D:421:ALA:HB2	2.02	0.41
1:A:381:LEU:N	1:A:381:LEU:CD2	2.83	0.41
1:C:382:LEU:HD22	1:C:436:PRO:HG3	2.01	0.41
1:A:464:ARG:NH2	1:A:467:PHE:CZ	2.89	0.41
1:B:121:VAL:HG23	1:B:239:ALA:HB1	2.03	0.41
1:B:34:LYS:HE3	1:B:42:MET:HE2	2.01	0.41
1:D:432:ARG:HH11	1:D:432:ARG:HG2	1.85	0.41
1:C:451:GLN:O	1:C:452:SER:C	2.57	0.41
1:D:96:ALA:C	1:D:101:GLN:HE22	2.16	0.41
1:A:459:LEU:CD1	1:A:459:LEU:C	2.89	0.41
1:B:148:LEU:HD13	1:B:199:TYR:CZ	2.55	0.41
1:D:36:LEU:HD23	1:D:70:GLN:OE1	2.20	0.41
1:A:251:LEU:O	1:A:255:LEU:HG	2.20	0.41
1:C:393:ARG:HG3	1:C:396:PRO:HD3	1.98	0.41
1:C:402:HIS:C	1:C:404:LEU:H	2.23	0.41
1:B:148:LEU:HD21	1:B:202:ARG:NH2	2.35	0.41
1:A:231:VAL:HA	1:A:267:ALA:O	2.20	0.41
1:C:237:GLY:O	1:C:239:ALA:N	2.54	0.41
1:D:129:LEU:HD21	1:D:310:GLY:CA	2.50	0.41
1:B:451:GLN:O	1:B:455:LEU:HG	2.21	0.41
1:D:352:VAL:O	1:D:353:ASP:O	2.38	0.41
1:C:211:LEU:N	1:C:212:PRO:CD	2.84	0.41
1:C:35:GLN:O	1:C:39:LEU:HG	2.21	0.41
1:B:108:TRP:CH2	1:B:139:LYS:HE2	2.56	0.41
1:B:48:ARG:O	1:B:49:LEU:HD23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:MET:SD	1:C:144:SER:OG	2.78	0.41
1:D:400:VAL:HG13	1:D:451:GLN:HG2	2.01	0.41
1:B:149:GLY:O	1:B:402:HIS:HE1	2.04	0.41
1:B:84:ASP:OD2	1:B:84:ASP:C	2.59	0.41
1:A:108:TRP:CZ3	1:A:177:LEU:HB2	2.56	0.41
1:A:305:LEU:HD21	1:A:472:PRO:HG2	2.01	0.41
1:D:312:ALA:O	1:D:316:LEU:HB2	2.20	0.41
1:D:54:ILE:HG23	1:D:91:LEU:CD1	2.50	0.41
1:A:50:SER:O	1:A:54:ILE:HG13	2.20	0.41
1:A:289:GLU:OE2	1:A:299:PRO:HG2	2.20	0.41
1:C:270:LEU:O	1:C:474:ALA:HB3	2.20	0.41
1:D:368:ARG:C	1:D:370:GLN:N	2.71	0.41
1:B:283:HIS:HB2	1:B:417:LEU:HA	2.03	0.41
1:C:249:ARG:HG2	1:C:249:ARG:NH1	2.35	0.41
1:D:63:ASN:HD22	1:D:63:ASN:H	1.66	0.41
1:A:478:LEU:HB3	1:A:479:PRO:HD2	2.02	0.41
1:D:410:ARG:O	1:D:413:GLU:HB3	2.21	0.41
1:D:383:ALA:HA	1:D:384:PRO:HD2	1.95	0.41
1:A:331:ALA:HA	1:A:334:LEU:HD12	2.02	0.41
1:B:293:CYS:O	1:B:334:LEU:HD22	2.21	0.41
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.81	0.41
1:B:408:ARG:CG	1:B:413:GLU:HG3	2.31	0.41
1:C:191:LEU:O	1:C:192:VAL:HG22	2.19	0.41
1:A:265:ARG:HD2	1:A:316:LEU:HD13	2.02	0.41
1:A:108:TRP:O	1:A:109:ARG:C	2.59	0.41
1:C:244:ASN:HB3	1:C:247:GLN:CB	2.51	0.41
1:D:378:GLN:HG2	1:D:441:HIS:ND1	2.36	0.41
1:D:331:ALA:O	1:D:334:LEU:HB2	2.21	0.41
1:A:115:LYS:HG2	1:A:129:LEU:HD12	2.02	0.41
1:A:313:LEU:HA	1:A:313:LEU:HD23	1.84	0.41
1:C:129:LEU:HA	1:C:129:LEU:HD23	1.85	0.41
1:B:211:LEU:N	1:B:212:PRO:HD2	2.36	0.41
1:C:401:LEU:HD22	1:C:401:LEU:N	2.36	0.41
1:D:416:ARG:HB3	1:D:443:ASP:OD1	2.21	0.41
1:A:125:VAL:HG23	1:A:277:LEU:CD1	2.51	0.41
1:D:104:TRP:O	1:D:109:ARG:NH1	2.54	0.41
1:B:127:LEU:HA	1:B:127:LEU:HD23	1.83	0.41
1:C:256:VAL:CG2	1:C:266:VAL:HG23	2.51	0.40
1:C:83:MET:CB	1:C:87:GLU:CD	2.90	0.40
1:A:425:VAL:HG13	1:A:437:TRP:HA	2.03	0.40
1:C:135:ALA:HA	1:C:342:ARG:HH12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLY:O	1:C:155:LEU:HB2	2.21	0.40
1:D:393:ARG:NH2	1:D:457:GLU:HG2	2.36	0.40
1:D:382:LEU:HD22	1:D:434:GLY:O	2.21	0.40
1:D:141:PRO:HG2	1:D:225:GLU:OE1	2.21	0.40
1:A:192:VAL:N	1:A:193:PRO:CD	2.84	0.40
1:B:112:LEU:HA	1:B:139:LYS:O	2.20	0.40
1:D:381:LEU:HB3	1:D:437:TRP:HE1	1.86	0.40
1:B:147:GLY:N	1:B:153:GLY:HA3	2.36	0.40
1:D:288:GLU:HG2	1:D:372:LEU:CD1	2.51	0.40
1:C:329:ARG:O	1:C:329:ARG:HD2	2.21	0.40
1:C:140:VAL:HA	1:C:141:PRO:HD2	2.02	0.40
1:C:188:SER:C	1:C:190:GLN:N	2.75	0.40
1:B:402:HIS:CG	1:B:407:GLY:HA3	2.57	0.40
1:A:393:ARG:NH2	1:B:178:ASP:OD2	2.54	0.40
1:B:36:LEU:HD23	1:B:39:LEU:HD12	2.04	0.40
1:D:155:LEU:HD23	1:D:155:LEU:HA	1.83	0.40
1:A:169:SER:O	1:A:170:PRO:C	2.58	0.40
1:B:122:GLY:HA2	1:B:286:GLU:OE2	2.21	0.40
1:C:113:VAL:CB	1:C:313:LEU:HD11	2.48	0.40
1:A:205:THR:O	1:A:205:THR:CG2	2.69	0.40
1:B:341:GLY:O	1:B:342:ARG:C	2.60	0.40
1:A:285:LEU:CD2	1:A:441:HIS:HD2	2.34	0.40
1:D:192:VAL:N	1:D:193:PRO:HD3	2.36	0.40
1:B:63:ASN:HD21	1:B:65:SER:HG	1.57	0.40
1:B:393:ARG:HB3	1:B:396:PRO:HD2	2.03	0.40
1:C:294:MET:HB3	1:C:340:LEU:CB	2.42	0.40
1:B:132:ALA:O	1:B:135:ALA:N	2.53	0.40
1:C:356:LEU:O	1:C:360:LEU:HG	2.22	0.40
1:B:313:LEU:HA	1:B:313:LEU:HD23	1.71	0.40
1:B:191:LEU:O	1:B:192:VAL:C	2.60	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	447/482 (93%)	383 (86%)	53 (12%)	11 (2%)	7 34
1	B	444/482 (92%)	386 (87%)	52 (12%)	6 (1%)	14 51
1	C	441/482 (92%)	371 (84%)	52 (12%)	18 (4%)	3 20
1	D	439/482 (91%)	362 (82%)	62 (14%)	15 (3%)	5 25
All	All	1771/1928 (92%)	1502 (85%)	219 (12%)	50 (3%)	6 30

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	119	GLY
1	A	295	ASP
1	A	376	ARG
1	A	411	ALA
1	B	112	LEU
1	C	35	GLN
1	C	109	ARG
1	C	382	LEU
1	C	425	VAL
1	D	364	SER
1	D	365	PRO
1	D	369	ARG
1	D	414	PRO
1	D	464	ARG
1	A	238	GLY
1	B	152	GLY
1	B	389	VAL
1	C	238	GLY
1	C	384	PRO
1	D	82	GLY
1	D	106	GLU
1	D	124	LYS
1	A	187	GLN
1	A	446	ALA
1	B	433	ARG
1	C	34	LYS
1	C	226	GLY
1	C	386	ASP
1	D	203	ASP

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Mol	Chain	Res	Type
1	A	33	PRO
1	C	276	PRO
1	C	376	ARG
1	D	98	SER
1	A	257	GLY
1	C	245	GLN
1	C	295	ASP
1	C	354	PRO
1	D	204	VAL
1	D	445	PRO
1	D	462	SER
1	B	141	PRO
1	C	243	PRO
1	C	445	PRO
1	A	224	VAL
1	C	82	GLY
1	D	351	GLY
1	D	170	PRO
1	B	257	GLY
1	C	414	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	334/359 (93%)	292 (87%)	42 (13%)	5 24
1	B	334/359 (93%)	290 (87%)	44 (13%)	5 22
1	C	332/359 (92%)	304 (92%)	28 (8%)	14 45
1	D	328/359 (91%)	294 (90%)	34 (10%)	9 32
All	All	1328/1436 (92%)	1180 (89%)	148 (11%)	8 29

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU

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Mol	Chain	Res	Type
1	A	43	LYS
1	A	63	ASN
1	A	79	ARG
1	A	85	LEU
1	A	92	THR
1	A	95	LEU
1	A	97	GLN
1	A	101	GLN
1	A	110	GLN
1	A	115	LYS
1	A	124	LYS
1	A	144	SER
1	A	159	GLU
1	A	174	GLN
1	A	179	GLN
1	A	192	VAL
1	A	203	ASP
1	A	211	LEU
1	A	242	PHE
1	A	244	ASN
1	A	273	MET
1	A	277	LEU
1	A	285	LEU
1	A	292	LEU
1	A	295	ASP
1	A	304	ASP
1	A	316	LEU
1	A	319	HIS
1	A	362	SER
1	A	369	ARG
1	A	379	GLU
1	A	381	LEU
1	A	391	LEU
1	A	410	ARG
1	A	431	LEU
1	A	432	ARG
1	A	438	LEU
1	A	453	ARG
1	A	456	GLN
1	A	460	VAL
1	A	463	ASP
1	B	38	GLU

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Mol	Chain	Res	Type
1	B	43	LYS
1	B	51	GLU
1	B	63	ASN
1	B	79	ARG
1	B	91	LEU
1	B	100	GLN
1	B	103	GLU
1	B	108	TRP
1	B	115	LYS
1	B	124	LYS
1	B	129	LEU
1	B	171	GLU
1	B	174	GLN
1	B	175	VAL
1	B	187	GLN
1	B	211	LEU
1	B	223	LEU
1	B	224	VAL
1	B	230	LEU
1	B	249	ARG
1	B	256	VAL
1	B	265	ARG
1	B	270	LEU
1	B	277	LEU
1	B	279	ARG
1	B	295	ASP
1	B	305	LEU
1	B	316	LEU
1	B	340	LEU
1	B	345	ARG
1	B	356	LEU
1	B	360	LEU
1	B	374	ARG
1	B	386	ASP
1	B	391	LEU
1	B	401	LEU
1	B	408	ARG
1	B	409	SER
1	B	410	ARG
1	B	431	LEU
1	B	457	GLU
1	B	459	LEU

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Mol	Chain	Res	Type
1	B	464	ARG
1	C	41	ARG
1	C	49	LEU
1	C	79	ARG
1	C	81	ARG
1	C	83	MET
1	C	91	LEU
1	C	97	GLN
1	C	106	GLU
1	C	115	LYS
1	C	124	LYS
1	C	136	CYS
1	C	214	ILE
1	C	230	LEU
1	C	265	ARG
1	C	273	MET
1	C	305	LEU
1	C	313	LEU
1	C	329	ARG
1	C	369	ARG
1	C	386	ASP
1	C	388	THR
1	C	397	LEU
1	C	415	LEU
1	C	430	ARG
1	C	431	LEU
1	C	442	ARG
1	C	463	ASP
1	C	464	ARG
1	D	41	ARG
1	D	43	LYS
1	D	51	GLU
1	D	63	ASN
1	D	79	ARG
1	D	101	GLN
1	D	103	GLU
1	D	109	ARG
1	D	115	LYS
1	D	140	VAL
1	D	159	GLU
1	D	167	ILE
1	D	244	ASN

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Mol	Chain	Res	Type
1	D	245	GLN
1	D	277	LEU
1	D	305	LEU
1	D	313	LEU
1	D	316	LEU
1	D	342	ARG
1	D	350	GLN
1	D	391	LEU
1	D	393	ARG
1	D	401	LEU
1	D	408	ARG
1	D	413	GLU
1	D	415	LEU
1	D	416	ARG
1	D	426	ASP
1	D	456	GLN
1	D	459	LEU
1	D	463	ASP
1	D	464	ARG
1	D	467	PHE
1	D	475	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	97	GLN
1	A	100	GLN
1	A	101	GLN
1	A	110	GLN
1	A	168	GLN
1	A	179	GLN
1	A	244	ASN
1	A	319	HIS
1	A	350	GLN
1	A	378	GLN
1	A	429	GLN
1	A	456	GLN
1	B	63	ASN
1	B	97	GLN
1	B	100	GLN
1	B	101	GLN

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Mol	Chain	Res	Type
1	B	187	GLN
1	B	245	GLN
1	B	319	HIS
1	B	350	GLN
1	B	378	GLN
1	B	456	GLN
1	C	97	GLN
1	C	101	GLN
1	C	111	GLN
1	C	165	ASN
1	C	168	GLN
1	C	244	ASN
1	C	247	GLN
1	C	319	HIS
1	C	350	GLN
1	C	429	GLN
1	D	35	GLN
1	D	63	ASN
1	D	67	GLN
1	D	93	GLN
1	D	97	GLN
1	D	244	ASN
1	D	245	GLN
1	D	323	GLN
1	D	325	GLN
1	D	350	GLN
1	D	456	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 (i)

1 ligand is 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	GOL	B	1481	-	5,5,5	4.64	5 (100%)	5,5,5	5.76	3 (60%)

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	GOL	B	1481	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1481	GOL	C3-C2	-7.60	1.23	1.52
2	B	1481	GOL	C1-C2	-2.87	1.41	1.52
2	B	1481	GOL	O2-C2	-2.36	1.36	1.43
2	B	1481	GOL	O3-C3	3.81	1.58	1.42
2	B	1481	GOL	O1-C1	4.66	1.62	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1481	GOL	O1-C1-C2	3.30	126.19	110.18
2	B	1481	GOL	O2-C2-C3	6.57	138.76	108.65
2	B	1481	GOL	O3-C3-C2	10.56	161.38	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	449/482 (93%)	-0.36	1 (0%)	95	87	15, 19, 40, 57	0
1	B	448/482 (92%)	-0.33	3 (0%)	89	70	15, 18, 40, 66	0
1	C	445/482 (92%)	-0.13	4 (0%)	85	64	15, 33, 56, 68	0
1	D	445/482 (92%)	-0.14	3 (0%)	89	70	15, 33, 58, 68	0
All	All	1787/1928 (92%)	-0.24	11 (0%)	90	73	15, 25, 53, 68	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	GLY	4.7
1	B	480	PRO	3.3
1	B	481	GLN	2.8
1	C	83	MET	2.5
1	C	381	LEU	2.4
1	C	378	GLN	2.4
1	D	435	THR	2.3
1	B	108	TRP	2.3
1	D	364	SER	2.2
1	C	431	LEU	2.1
1	A	32	GLU	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	GOL	B	1481	6/6	0.87	0.26	4.53	24,28,29,29	0

6.5 Other polymers

There are no such residues in this entry.