Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2021 – 11:03 AM EDT

PDB ID	:	3IB9
Title	:	Propionyl-CoA Carboxylase Beta Subunit, D422L
Authors	:	Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Pham, H.; Melgar, M.M.
Deposited on	:	2009-07-15
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

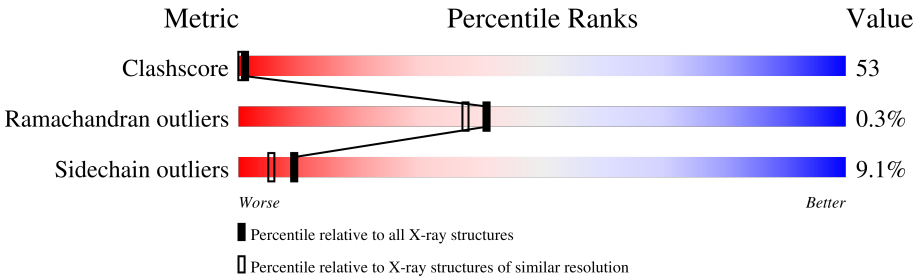
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	530	42% 51% 5% •
1	B	530	42% 51% 6% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8285 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.

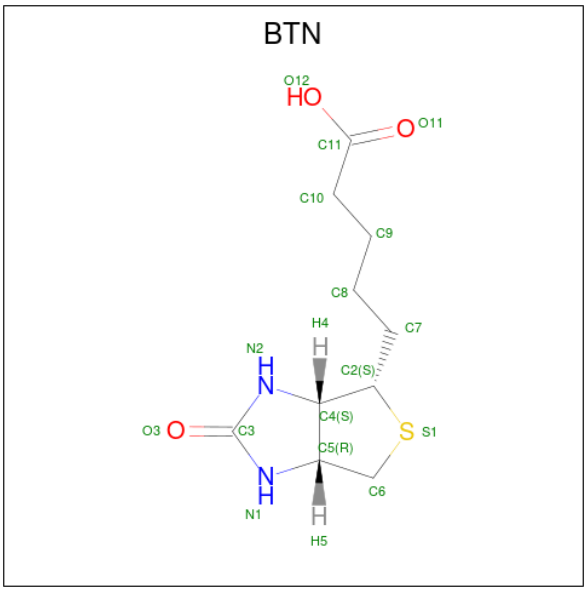
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			
1	B	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	LEU	ASP	engineered mutation	UNP Q9X4K7
B	422	LEU	ASP	engineered mutation	UNP Q9X4K7

- Molecule 2 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

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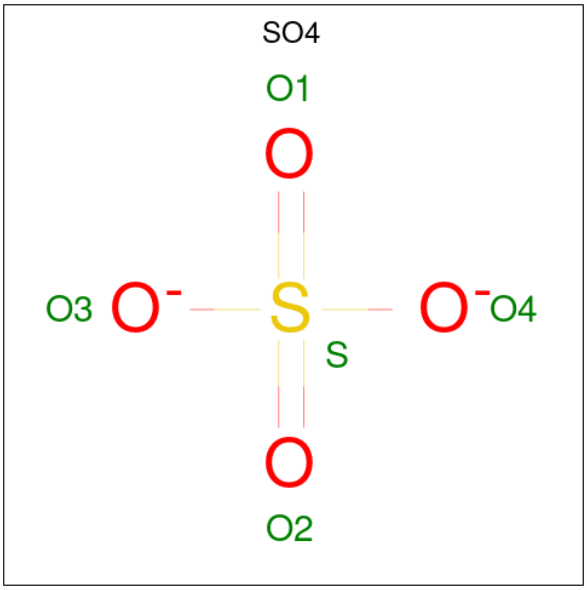
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

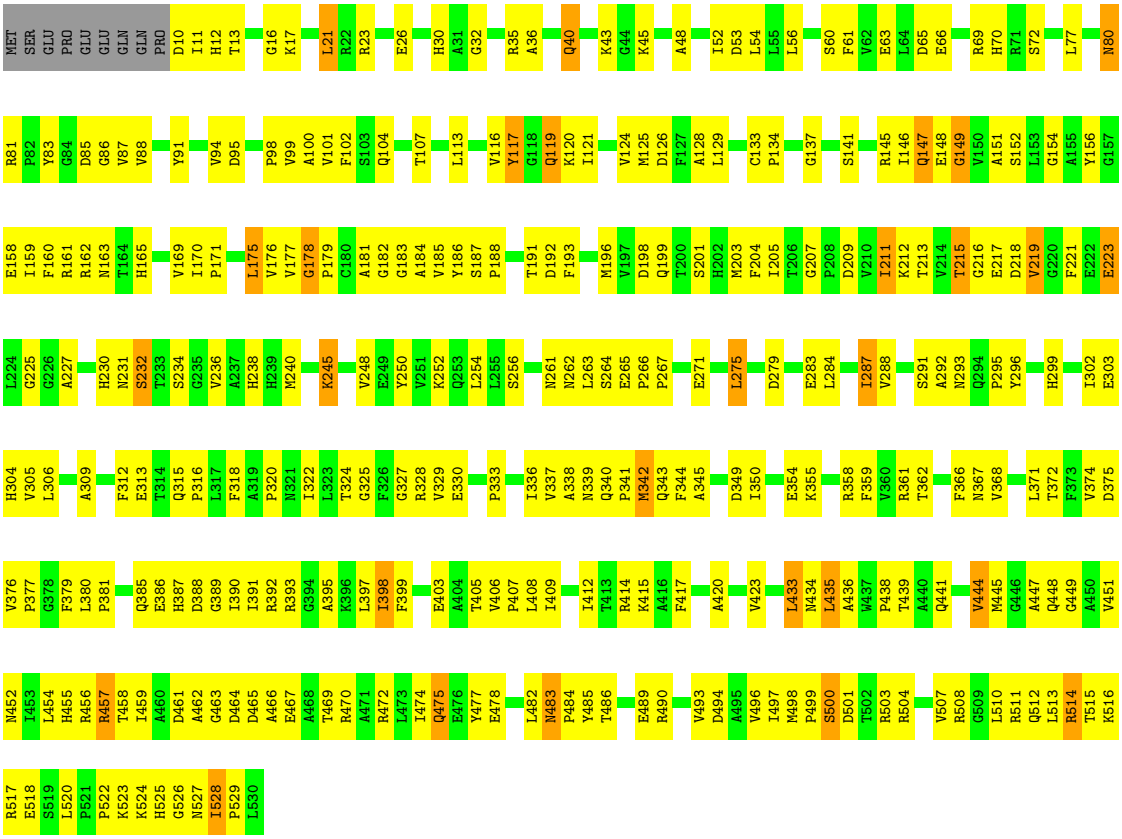
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	172	Total	O	0	0
			172	172		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

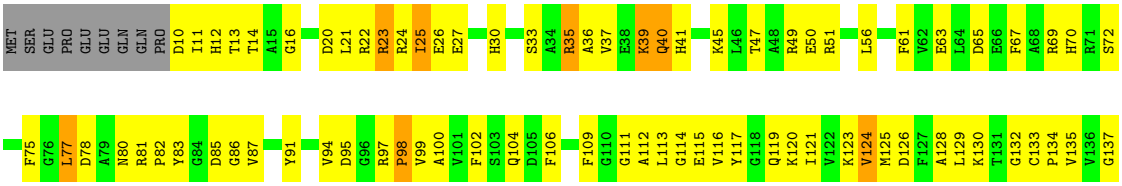
• Molecule 1: Propionyl-CoA carboxylase complex B subunit

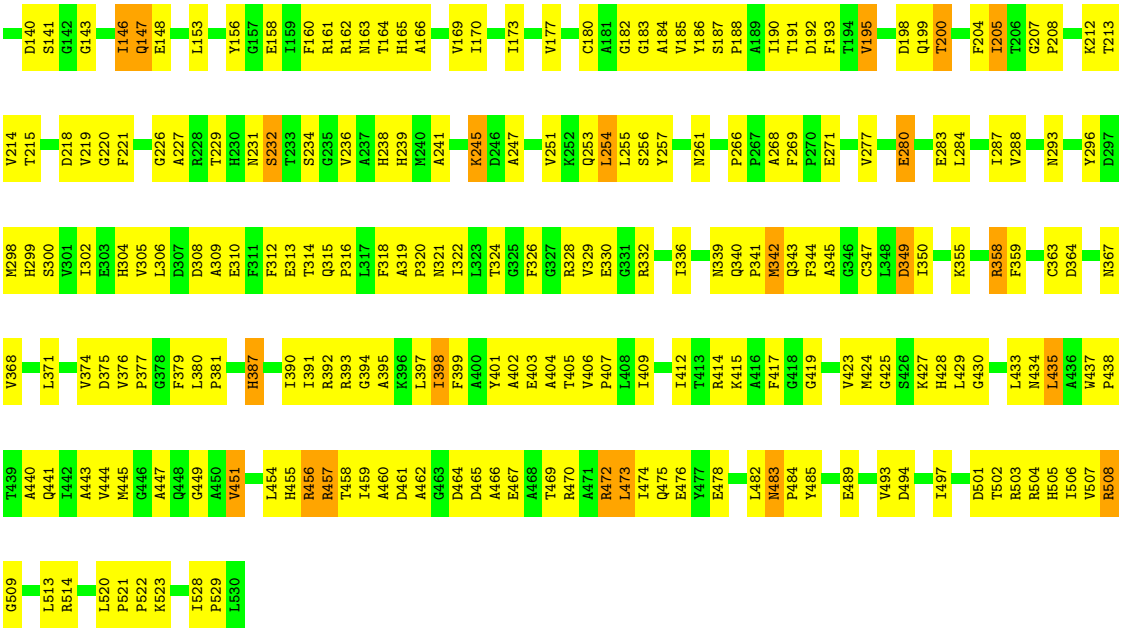
Chain A:



• Molecule 1: Propionyl-CoA carboxylase complex B subunit

Chain B:




D140 S141 G142 G143 I146 Q147 E148 L153 Y156 G157 E158 I159 F160 R161 R162 N163 T164 H165 A166 V169 I170 I173 V177 C180 A181 G182 G183 A184 V185 Y186 S187 P188 A189 I190 T191 D192 F193 T194 V195 D198 Q199 T200 F204 I205 T206 G207 P208 K212 T213
V214 T215 D218 V219 G220 F221 G226 A227 R228 T229 H230 N231 S232 T233 S234 G235 V236 A237 H238 H239 M240 A241 K245 D246 A247 V251 K252 Q253 L254 L255 S256 Y257 N261 P266 P267 A268 F269 P270 E271 V277 E280 E283 L284 I287 V288 N293 Y296 D297
M298 H299 S300 V301 I302 E303 H304 V305 L306 D307 D308 A309 E310 F311 F312 E313 T314 Q315 P316 L317 F318 A319 P320 N321 I322 L323 T324 G325 F326 G327 R328 V329 E330 G331 R332 I336 N339 Q340 P341 M342 Q343 F344 A345 G346 C347 L348 D349 I350 K355 R358 F359 C363 D364 N367
V368 L371 V374 D375 V376 P377 G378 F379 L380 P381 H387 I390 I391 R392 R393 G394 A395 K396 L397 I398 F399 A400 Y401 A402 E403 A404 T405 V406 P407 L408 I409 I412 T413 R414 K415 A416 F417 G418 G419 V423 M424 G425 S426 K427 H428 L429 G430 L433 N434 L435 A436 W437 P438
T439 A440 Q441 I442 A443 V444 M445 G446 A447 Q448 G449 A450 V451 L454 H455 R456 R457 T458 I459 A460 D461 A462 G463 D464 D465 A466 E467 A468 T469 R470 A471 R472 L473 I474 Q475 E476 Y477 E478 L482 M483 P484 Y485 E489 V493 D494 I497 D501 T502 R503 R504 H505 I506 V507 R508
G509 L513 R514 L520 P521 P522 K523 I528 P529 L530

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	168.49Å 168.49Å 80.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 29.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.00) 70.8 (29.60-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-3.70 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.274 0.317 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8285	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BTN

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	0.23	0/4032	0.49	2/5478 (0.0%)
1	B	0.24	0/4032	0.49	0/5478
All	All	0.24	0/8064	0.49	2/10956 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	GLY	C-N-CD	-5.88	107.67	120.60
1	A	149	GLY	N-CA-C	5.04	125.69	113.10

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	3952	0	3887	461	0
1	B	3952	0	3887	432	0
2	A	16	0	15	2	0
2	B	16	0	15	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	167	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	172	0	0	13	0
All	All	8285	0	7804	842	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 53.

All (842) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HB	1:A:117:TYR:CE2	1.33	1.57
1:A:456:ARG:NH1	1:A:457:ARG:HH22	1.30	1.29
1:A:87:VAL:HB	1:A:117:TYR:CD2	1.68	1.26
1:B:113:LEU:HD13	1:B:156:TYR:CE1	1.72	1.25
1:A:456:ARG:NH1	1:A:457:ARG:NH2	1.91	1.18
1:A:212:LYS:HD3	1:A:218:ASP:OD1	1.40	1.18
1:A:397:LEU:HD23	1:A:423:VAL:CG1	1.73	1.17
1:B:113:LEU:HD22	1:B:156:TYR:CE1	1.81	1.15
1:A:87:VAL:CB	1:A:117:TYR:CE2	2.30	1.15
1:B:113:LEU:CD1	1:B:156:TYR:HE1	1.62	1.13
1:A:362:THR:O	1:A:366:PHE:HD2	1.33	1.11
1:B:21:LEU:O	1:B:25:ILE:HG22	1.50	1.11
1:B:193:PHE:HA	1:B:238:HIS:CE1	1.87	1.10
1:B:457:ARG:HH11	1:B:457:ARG:CG	1.65	1.10
1:B:397:LEU:HD23	1:B:423:VAL:CG1	1.82	1.09
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.34	1.09
1:A:146:ILE:HG22	1:B:454:LEU:HD11	1.35	1.08
1:A:203:MET:HB2	1:A:230:HIS:NE2	1.68	1.08
1:A:160:PHE:HE1	1:A:187:SER:HB2	1.18	1.08
1:B:113:LEU:HB3	1:B:156:TYR:OH	1.53	1.08
1:A:104:GLN:HG2	1:A:117:TYR:OH	1.54	1.07
1:A:478:GLU:HA	1:A:482:LEU:CD1	1.84	1.07
1:B:349:ASP:CB	1:B:380:LEU:HD12	1.85	1.07
1:A:390:ILE:HG21	1:B:205:ILE:HD11	1.12	1.07
1:A:478:GLU:CA	1:A:482:LEU:HD13	1.85	1.07
1:A:87:VAL:CB	1:A:117:TYR:CD2	2.38	1.05
1:B:392:ARG:HG3	1:B:393:ARG:HG3	1.39	1.05
1:A:146:ILE:CG2	1:B:454:LEU:HD11	1.86	1.04
1:B:113:LEU:HD13	1:B:156:TYR:HE1	0.89	1.04
1:A:478:GLU:HA	1:A:482:LEU:HD13	1.04	1.03
1:A:87:VAL:HB	1:A:117:TYR:HE2	1.21	1.02
1:B:397:LEU:HD23	1:B:423:VAL:HG11	1.39	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:HH11	1:B:457:ARG:HG2	0.88	1.02
1:B:509:GLY:O	1:B:513:LEU:HG	1.60	1.00
1:A:215:THR:HG21	4:A:575:HOH:O	1.62	0.99
1:B:347:CYS:SG	1:B:377:PRO:HG2	2.01	0.99
1:A:397:LEU:HD23	1:A:423:VAL:HG11	1.44	0.99
1:A:160:PHE:CE1	1:A:187:SER:HB2	1.98	0.98
1:A:32:GLY:HA3	1:A:107:THR:HG21	1.43	0.98
1:B:349:ASP:HB2	1:B:380:LEU:HD12	1.42	0.98
1:A:10:ASP:O	1:A:16:GLY:HA3	1.63	0.97
1:A:32:GLY:HA3	1:A:107:THR:CG2	1.94	0.97
1:A:395:ALA:O	1:A:398:ILE:HG23	1.63	0.96
1:A:113:LEU:HD12	1:A:117:TYR:HD1	1.30	0.96
1:B:87:VAL:HB	1:B:117:TYR:CE2	2.00	0.96
1:B:257:TYR:CE1	1:B:328:ARG:NH1	2.34	0.95
1:B:98:PRO:O	1:B:99:VAL:HG23	1.67	0.94
1:A:231:ASN:OD1	1:A:240:MET:HB2	1.66	0.94
1:A:405:THR:HG21	1:A:518:GLU:O	1.66	0.94
1:B:326:PHE:HE1	1:B:363:CYS:HG	0.94	0.94
1:A:377:PRO:HG3	1:A:415:LYS:HD3	1.50	0.93
1:A:392:ARG:HG3	1:A:393:ARG:HG3	1.48	0.93
1:A:390:ILE:HG21	1:B:205:ILE:CD1	1.96	0.93
1:A:99:VAL:HG22	1:A:134:PRO:HB2	1.50	0.93
1:B:470:ARG:O	1:B:474:ILE:HG13	1.69	0.93
1:B:445:MET:HE2	1:B:449:GLY:C	1.88	0.93
1:B:198:ASP:OD1	1:B:199:GLN:HG2	1.67	0.93
1:A:362:THR:O	1:A:366:PHE:CD2	2.22	0.92
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.51	0.92
1:A:193:PHE:HA	1:A:238:HIS:CE1	2.04	0.92
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.50	0.92
1:A:451:VAL:HG21	1:A:474:ILE:HG12	1.51	0.91
1:B:440:ALA:O	1:B:484:PRO:HD3	1.71	0.91
1:B:200:THR:HG23	1:B:200:THR:O	1.70	0.91
1:B:113:LEU:CD2	1:B:156:TYR:CE1	2.54	0.91
1:A:380:LEU:HD22	1:A:381:PRO:HD2	1.49	0.90
1:A:467:GLU:HG3	1:A:470:ARG:HH21	1.34	0.90
1:B:457:ARG:HG2	1:B:457:ARG:NH1	1.62	0.90
1:A:87:VAL:CG1	1:A:117:TYR:CD2	2.54	0.90
1:B:241:ALA:HB3	1:B:247:ALA:HB2	1.53	0.89
1:A:457:ARG:HH11	1:A:457:ARG:CG	1.85	0.88
1:B:409:ILE:HD11	1:B:513:LEU:HD12	1.54	0.88
1:A:196:MET:SD	1:A:203:MET:HE2	2.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:HB3	1:B:190:ILE:HG21	1.55	0.88
1:B:315:GLN:OE1	1:B:355:LYS:HG3	1.74	0.88
1:A:265:GLU:HG2	1:A:266:PRO:HD2	1.56	0.88
1:A:398:ILE:CD1	1:B:160:PHE:HB3	2.03	0.88
1:B:528:ILE:HG12	1:B:529:PRO:HD2	1.56	0.87
1:A:447:ALA:HB2	1:A:482:LEU:HD21	1.57	0.87
1:A:113:LEU:HD12	1:A:117:TYR:CD1	2.09	0.87
1:A:212:LYS:CD	1:A:218:ASP:OD1	2.23	0.87
1:A:147:GLN:H	1:A:147:GLN:HE21	1.15	0.87
1:B:113:LEU:CD1	1:B:156:TYR:CE1	2.47	0.87
1:B:528:ILE:CG1	1:B:529:PRO:HD2	2.04	0.86
1:A:397:LEU:CD2	1:A:423:VAL:CG1	2.53	0.86
1:A:456:ARG:HH11	1:A:457:ARG:HH22	0.86	0.86
1:A:391:ILE:HG13	4:A:602:HOH:O	1.75	0.86
1:A:405:THR:CG2	1:A:518:GLU:O	2.22	0.86
1:A:86:GLY:O	1:A:117:TYR:CE2	2.29	0.86
1:A:511:ARG:O	1:A:514:ARG:HG2	1.75	0.86
1:B:397:LEU:CD2	1:B:423:VAL:CG1	2.53	0.85
1:A:447:ALA:O	1:A:451:VAL:HG13	1.76	0.85
1:B:113:LEU:HB3	1:B:156:TYR:CZ	2.11	0.85
1:A:104:GLN:CG	1:A:117:TYR:OH	2.25	0.85
1:A:451:VAL:HG11	1:A:474:ILE:HA	1.59	0.85
1:B:245:LYS:HZ3	1:B:245:LYS:HB2	1.42	0.85
1:A:85:ASP:O	1:A:117:TYR:HB2	1.77	0.84
1:A:459:ILE:CD1	1:A:470:ARG:HB2	2.06	0.84
1:B:25:ILE:HD12	4:B:644:HOH:O	1.77	0.84
1:B:113:LEU:HG	1:B:117:TYR:CD1	2.11	0.84
1:A:117:TYR:CD1	1:A:117:TYR:O	2.30	0.84
1:B:70:HIS:CE1	1:B:81:ARG:HG2	2.14	0.83
1:A:503:ARG:O	1:A:507:VAL:HG23	1.80	0.82
1:B:98:PRO:O	1:B:99:VAL:CG2	2.27	0.82
1:B:269:PHE:O	1:B:269:PHE:CD2	2.32	0.82
1:B:302:ILE:O	1:B:305:VAL:HG22	1.80	0.82
1:A:456:ARG:HH11	1:A:457:ARG:NH2	1.60	0.82
1:A:315:GLN:OE1	1:A:355:LYS:HG3	1.79	0.81
1:B:102:PHE:CZ	1:B:137:GLY:HA3	2.14	0.81
1:A:287:ILE:HG12	1:A:287:ILE:O	1.79	0.81
1:A:341:PRO:HG3	1:A:375:ASP:OD2	1.81	0.81
1:B:170:ILE:HG22	1:B:261:ASN:HB3	1.62	0.81
1:B:455:HIS:NE2	1:B:473:LEU:HG	1.95	0.81
1:B:86:GLY:O	1:B:117:TYR:HE2	1.64	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLY:O	1:B:444:VAL:HG23	1.81	0.81
1:A:113:LEU:O	1:A:145:ARG:HB2	1.79	0.80
1:A:70:HIS:HD2	1:A:72:SER:H	1.30	0.80
1:B:326:PHE:HE1	1:B:363:CYS:SG	2.05	0.80
1:B:398:ILE:HG13	1:B:399:PHE:N	1.95	0.80
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.63	0.80
1:B:475:GLN:HA	1:B:478:GLU:OE1	1.82	0.80
1:A:520:LEU:HD22	1:B:165:HIS:CD2	2.16	0.79
1:B:200:THR:O	1:B:200:THR:CG2	2.30	0.79
1:A:98:PRO:O	1:A:99:VAL:HG23	1.83	0.79
1:A:149:GLY:O	1:B:444:VAL:CG2	2.30	0.79
1:A:371:LEU:HD21	1:A:510:LEU:HD11	1.65	0.79
1:A:113:LEU:HD23	1:A:156:TYR:CZ	2.18	0.79
1:B:23:ARG:O	1:B:23:ARG:CD	2.31	0.78
1:A:113:LEU:HD23	1:A:156:TYR:CE2	2.18	0.78
1:B:113:LEU:CG	1:B:156:TYR:CE1	2.67	0.78
1:B:115:GLU:HG2	1:B:119:GLN:OE1	1.82	0.78
1:A:145:ARG:HD2	1:A:148:GLU:OE2	1.82	0.78
1:A:146:ILE:HG22	1:B:454:LEU:CD1	2.13	0.78
1:A:474:ILE:O	1:A:478:GLU:HG3	1.84	0.78
1:B:445:MET:HE3	1:B:449:GLY:HA3	1.66	0.78
1:A:380:LEU:HD13	1:A:380:LEU:C	2.05	0.77
1:B:35:ARG:O	1:B:39:LYS:HG2	1.85	0.77
1:A:398:ILE:HG13	1:A:399:PHE:N	1.98	0.77
1:A:147:GLN:H	1:A:147:GLN:NE2	1.81	0.77
1:B:415:LYS:HG2	1:B:417:PHE:HE2	1.49	0.77
1:A:362:THR:HG23	1:A:366:PHE:HE2	1.50	0.76
1:A:470:ARG:O	1:A:474:ILE:HG13	1.85	0.76
1:A:302:ILE:O	1:A:305:VAL:HG22	1.85	0.76
1:B:379:PHE:O	1:B:381:PRO:HD3	1.84	0.76
1:B:23:ARG:HD2	1:B:27:GLU:OE1	1.85	0.76
1:B:121:ILE:O	1:B:125:MET:HG3	1.84	0.76
1:A:160:PHE:HB3	1:B:398:ILE:HD13	1.65	0.76
1:B:316:PRO:HD2	4:B:547:HOH:O	1.85	0.76
1:A:467:GLU:HG3	1:A:470:ARG:NH2	2.01	0.75
1:A:350:ILE:H	1:A:385:GLN:HE22	1.34	0.75
1:A:459:ILE:HD13	1:A:470:ARG:HB2	1.66	0.75
1:A:10:ASP:O	1:A:16:GLY:CA	2.34	0.75
1:A:457:ARG:HH11	1:A:457:ARG:HG2	1.49	0.75
1:A:113:LEU:HD22	1:A:156:TYR:CE1	2.21	0.75
1:A:339:ASN:HB2	1:A:375:ASP:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ILE:HD11	1:B:513:LEU:CD1	2.16	0.75
1:B:113:LEU:HD22	1:B:156:TYR:CD1	2.22	0.74
1:B:445:MET:CE	1:B:449:GLY:C	2.55	0.74
1:A:520:LEU:CD2	1:B:165:HIS:NE2	2.50	0.74
1:A:87:VAL:HG12	1:A:117:TYR:CD2	2.21	0.74
1:A:275:LEU:HD21	1:A:507:VAL:HG11	1.68	0.74
1:B:70:HIS:CD2	4:B:566:HOH:O	2.39	0.74
1:A:513:LEU:O	1:A:516:LYS:N	2.20	0.74
1:A:10:ASP:O	1:A:10:ASP:OD1	2.06	0.74
1:A:187:SER:HB3	1:A:188:PRO:CD	2.17	0.74
1:B:70:HIS:CE1	1:B:77:LEU:O	2.41	0.74
1:A:320:PRO:HB2	1:A:343:GLN:HG3	1.68	0.74
1:B:326:PHE:CE1	1:B:363:CYS:SG	2.80	0.74
1:A:227:ALA:HB1	1:A:240:MET:HG3	1.70	0.74
1:A:154:GLY:HA2	1:B:428:HIS:CE1	2.21	0.73
1:B:104:GLN:HG2	1:B:117:TYR:OH	1.88	0.73
1:B:528:ILE:HG12	1:B:529:PRO:CD	2.18	0.73
1:A:316:PRO:HD2	4:A:600:HOH:O	1.89	0.73
1:A:469:THR:O	1:A:472:ARG:HB3	1.89	0.73
1:B:287:ILE:HG23	1:B:288:VAL:N	2.03	0.73
1:A:265:GLU:HG2	1:A:266:PRO:CD	2.19	0.73
1:A:405:THR:O	1:A:516:LYS:CE	2.37	0.72
1:A:146:ILE:CG2	1:B:454:LEU:CD1	2.65	0.72
1:B:158:GLU:OE2	1:B:161:ARG:NH1	2.22	0.72
1:A:513:LEU:O	1:A:515:THR:N	2.23	0.72
1:B:277:VAL:HG23	1:B:277:VAL:O	1.89	0.72
1:B:23:ARG:O	1:B:23:ARG:HD2	1.89	0.72
1:B:87:VAL:HG12	1:B:117:TYR:CD2	2.25	0.72
1:B:113:LEU:HG	1:B:117:TYR:HD1	1.50	0.72
1:A:193:PHE:HD1	1:A:238:HIS:CD2	2.07	0.71
1:A:293:ASN:O	1:A:295:PRO:HD3	1.90	0.71
1:A:299:HIS:HE1	1:A:313:GLU:OE2	1.72	0.71
1:B:254:LEU:HD13	1:B:312:PHE:HE2	1.56	0.71
1:B:445:MET:HE2	1:B:449:GLY:O	1.90	0.71
1:B:339:ASN:ND2	1:B:424:MET:HE1	2.05	0.71
1:A:32:GLY:CA	1:A:107:THR:CG2	2.68	0.71
1:A:113:LEU:CD2	1:A:156:TYR:CE1	2.74	0.70
1:A:215:THR:HG23	1:A:215:THR:O	1.88	0.70
1:B:339:ASN:HD21	1:B:424:MET:HE1	1.56	0.70
1:B:451:VAL:HB	1:B:455:HIS:HD2	1.55	0.70
1:B:106:PHE:HB2	1:B:140:ASP:OD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:HD13	1:B:160:PHE:HB3	1.71	0.70
1:A:292:ALA:O	1:A:414:ARG:NH1	2.25	0.70
1:A:399:PHE:CD1	1:B:164:THR:HG23	2.27	0.70
1:A:504:ARG:HG2	1:A:508:ARG:HD2	1.72	0.70
1:B:80:ASN:C	1:B:82:PRO:HD3	2.13	0.70
1:A:196:MET:O	1:A:240:MET:HA	1.92	0.70
1:B:115:GLU:O	1:B:119:GLN:HG3	1.92	0.70
1:B:298:MET:HG3	1:B:298:MET:O	1.92	0.69
1:B:485:TYR:O	1:B:489:GLU:HG3	1.92	0.69
1:A:344:PHE:O	1:A:345:ALA:HB3	1.91	0.69
1:B:374:VAL:HB	1:B:412:ILE:HA	1.72	0.69
1:A:399:PHE:CE1	1:B:164:THR:HG23	2.27	0.69
1:B:349:ASP:HB3	1:B:380:LEU:HD12	1.72	0.69
1:B:193:PHE:HD1	1:B:238:HIS:CD2	2.09	0.69
1:B:102:PHE:CZ	1:B:137:GLY:CA	2.75	0.69
1:B:339:ASN:HD21	1:B:424:MET:CE	2.06	0.69
1:A:329:VAL:O	1:A:330:GLU:HB2	1.92	0.69
1:A:354:GLU:OE2	1:B:392:ARG:NH1	2.21	0.69
1:B:10:ASP:CG	1:B:11:ILE:H	1.94	0.69
1:A:165:HIS:CD2	1:B:520:LEU:HD22	2.28	0.69
1:A:231:ASN:O	1:A:318:PHE:HB2	1.93	0.69
1:B:349:ASP:CB	1:B:380:LEU:CD1	2.68	0.69
1:B:22:ARG:HA	1:B:25:ILE:CG2	2.22	0.69
1:A:36:ALA:HB3	1:A:107:THR:HG23	1.74	0.69
1:A:254:LEU:HD23	1:A:312:PHE:HE2	1.57	0.69
1:B:160:PHE:HE1	1:B:187:SER:HB2	1.57	0.69
1:B:447:ALA:O	1:B:451:VAL:HG13	1.92	0.69
1:A:266:PRO:HG2	1:A:368:VAL:HG22	1.76	0.68
1:A:397:LEU:CD2	1:A:423:VAL:HG12	2.23	0.68
1:A:266:PRO:CG	1:A:368:VAL:HG22	2.24	0.68
1:A:457:ARG:CG	1:A:457:ARG:NH1	2.52	0.68
1:A:524:LYS:HD3	4:B:697:HOH:O	1.93	0.68
1:A:367:ASN:HA	1:A:406:VAL:HG11	1.75	0.68
1:A:32:GLY:CA	1:A:107:THR:HG21	2.22	0.68
1:A:380:LEU:HD13	1:A:380:LEU:O	1.94	0.67
1:B:438:PRO:HD3	1:B:497:ILE:O	1.94	0.67
1:A:113:LEU:CD1	1:A:117:TYR:CD1	2.77	0.67
1:A:407:PRO:HB3	1:A:513:LEU:HD23	1.76	0.67
1:A:455:HIS:O	1:A:459:ILE:HG22	1.95	0.67
1:A:520:LEU:CD2	1:B:165:HIS:CE1	2.77	0.67
1:B:456:ARG:O	1:B:459:ILE:CG2	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:O	1:A:211:ILE:HG23	1.95	0.67
1:A:485:TYR:O	1:A:489:GLU:HG3	1.94	0.67
1:B:254:LEU:HD13	1:B:312:PHE:CE2	2.29	0.67
1:A:221:PHE:CB	2:A:5600:BTN:H81	2.24	0.67
1:A:120:LYS:O	1:A:124:VAL:HG23	1.94	0.67
1:A:339:ASN:CB	1:A:375:ASP:O	2.43	0.67
1:A:501:ASP:OD1	1:A:501:ASP:O	2.13	0.67
1:B:113:LEU:CB	1:B:156:TYR:OH	2.40	0.67
1:A:181:ALA:CB	1:A:204:PHE:CE1	2.78	0.66
1:B:231:ASN:HD21	1:B:239:HIS:N	1.93	0.66
1:B:241:ALA:CB	1:B:247:ALA:HB2	2.23	0.66
1:B:339:ASN:O	1:B:341:PRO:HD3	1.96	0.66
1:B:456:ARG:O	1:B:459:ILE:HG23	1.96	0.66
1:A:456:ARG:O	1:A:457:ARG:HG3	1.96	0.66
1:A:482:LEU:N	1:A:482:LEU:HD12	2.10	0.66
1:B:459:ILE:HD13	1:B:470:ARG:HB2	1.77	0.66
1:B:509:GLY:O	1:B:513:LEU:CG	2.41	0.66
1:B:349:ASP:HB3	1:B:380:LEU:CD1	2.26	0.66
1:B:11:ILE:HG23	1:B:12:HIS:N	2.10	0.66
1:B:407:PRO:HB3	1:B:513:LEU:HB3	1.77	0.66
1:A:406:VAL:HG12	4:B:625:HOH:O	1.95	0.66
1:B:287:ILE:CG2	1:B:288:VAL:N	2.59	0.66
1:A:85:ASP:OD2	1:A:116:VAL:HB	1.96	0.65
1:A:386:GLU:OE2	1:B:204:PHE:HA	1.96	0.65
1:B:392:ARG:CG	1:B:393:ARG:HG3	2.23	0.65
1:A:462:ALA:O	1:A:464:ASP:N	2.29	0.65
1:A:121:ILE:O	1:A:121:ILE:HG22	1.95	0.65
1:A:113:LEU:CD2	1:A:156:TYR:CZ	2.79	0.65
1:B:41:HIS:ND1	4:B:617:HOH:O	2.28	0.65
1:A:119:GLN:O	1:A:119:GLN:NE2	2.30	0.65
1:A:193:PHE:CD1	1:A:238:HIS:CD2	2.84	0.65
1:B:508:ARG:HD3	4:B:637:HOH:O	1.96	0.65
1:A:70:HIS:CE1	1:A:81:ARG:HG2	2.32	0.65
1:A:477:TYR:HD1	1:A:482:LEU:HD11	1.61	0.65
1:B:129:LEU:HD21	1:B:166:ALA:HB2	1.78	0.65
1:A:490:ARG:NH2	1:B:115:GLU:OE1	2.30	0.65
1:B:114:GLY:HA3	1:B:148:GLU:OE2	1.97	0.65
1:B:245:LYS:HB2	1:B:245:LYS:NZ	2.11	0.64
1:A:362:THR:CG2	1:A:366:PHE:CE2	2.81	0.64
1:B:23:ARG:O	1:B:23:ARG:NE	2.30	0.64
1:A:362:THR:HG23	1:A:366:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HD21	1:B:109:PHE:CE1	2.32	0.64
1:B:502:THR:O	1:B:506:ILE:HG12	1.97	0.64
1:B:347:CYS:SG	1:B:377:PRO:CG	2.83	0.64
1:B:113:LEU:HD22	1:B:156:TYR:CZ	2.33	0.64
1:A:392:ARG:HG3	1:A:393:ARG:CG	2.26	0.64
1:B:23:ARG:HH21	1:B:24:ARG:HG3	1.63	0.64
1:B:114:GLY:CA	1:B:148:GLU:OE2	2.45	0.64
1:B:257:TYR:HE1	1:B:328:ARG:NH1	1.94	0.64
1:B:336:ILE:HD13	1:B:371:LEU:HB2	1.79	0.64
1:B:402:ALA:HB2	1:B:429:LEU:HD22	1.78	0.64
1:B:528:ILE:HG13	1:B:529:PRO:HD2	1.78	0.63
1:A:520:LEU:HD22	1:B:165:HIS:NE2	2.11	0.63
1:A:126:ASP:OD1	1:A:162:ARG:HD3	1.97	0.63
1:B:457:ARG:HD3	1:B:457:ARG:N	2.14	0.63
1:B:23:ARG:C	1:B:23:ARG:HE	2.01	0.63
1:B:397:LEU:CD2	1:B:423:VAL:HG12	2.29	0.63
1:A:387:HIS:O	1:B:234:SER:CB	2.46	0.63
1:B:26:GLU:O	1:B:30:HIS:HD2	1.81	0.63
1:A:181:ALA:HB2	1:A:204:PHE:CE1	2.33	0.62
1:B:339:ASN:OD1	1:B:424:MET:HE2	1.99	0.62
1:B:86:GLY:O	1:B:117:TYR:CE2	2.50	0.62
1:A:403:GLU:HA	1:A:520:LEU:HD11	1.81	0.62
1:B:147:GLN:H	1:B:147:GLN:NE2	1.96	0.62
1:B:170:ILE:HG22	1:B:261:ASN:CB	2.30	0.62
1:A:374:VAL:HB	1:A:412:ILE:HA	1.80	0.62
1:B:455:HIS:O	1:B:457:ARG:N	2.32	0.62
1:B:417:PHE:CE1	1:B:443:ALA:HB3	2.34	0.62
1:A:87:VAL:HG12	1:A:117:TYR:HD2	1.65	0.62
1:A:32:GLY:HA3	1:A:107:THR:HG22	1.80	0.62
1:A:169:VAL:HA	1:A:262:ASN:ND2	2.15	0.62
1:A:459:ILE:HD11	1:A:470:ARG:HB2	1.82	0.62
1:B:455:HIS:CD2	1:B:473:LEU:HG	2.33	0.62
1:A:125:MET:CE	1:A:163:ASN:ND2	2.63	0.62
1:B:401:TYR:CD2	1:B:423:VAL:O	2.52	0.62
1:A:397:LEU:HD23	1:A:423:VAL:HG12	1.73	0.62
1:A:376:VAL:O	1:A:376:VAL:HG13	1.99	0.62
1:B:97:ARG:HB3	1:B:98:PRO:HD2	1.82	0.61
1:A:405:THR:O	1:A:516:LYS:NZ	2.32	0.61
1:A:86:GLY:O	1:A:117:TYR:CD2	2.53	0.61
1:A:117:TYR:CD1	1:A:117:TYR:C	2.74	0.61
1:A:528:ILE:HG12	1:A:529:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLN:CD	1:B:342:MET:HG3	2.21	0.61
1:B:462:ALA:C	1:B:464:ASP:N	2.52	0.61
1:A:117:TYR:O	1:A:117:TYR:CG	2.53	0.61
1:A:147:GLN:HE21	1:A:147:GLN:N	1.94	0.61
1:A:451:VAL:HG21	1:A:474:ILE:CG1	2.26	0.61
1:B:112:ALA:HA	1:B:143:GLY:O	2.01	0.60
1:A:362:THR:CG2	1:A:366:PHE:HE2	2.13	0.60
1:B:113:LEU:CG	1:B:156:TYR:HE1	2.06	0.60
1:B:193:PHE:CD1	1:B:238:HIS:CD2	2.88	0.60
1:A:36:ALA:CB	1:A:107:THR:HG23	2.31	0.60
1:A:392:ARG:CG	1:A:393:ARG:HG3	2.26	0.60
1:B:102:PHE:CE1	1:B:137:GLY:HA3	2.36	0.60
1:B:113:LEU:HG	1:B:117:TYR:CE1	2.36	0.60
1:A:32:GLY:CA	1:A:107:THR:HG22	2.31	0.60
1:A:525:HIS:ND1	1:A:526:GLY:O	2.35	0.60
1:A:21:LEU:O	1:A:21:LEU:HG	2.01	0.60
1:A:221:PHE:HB2	2:A:5600:BTN:H81	1.84	0.60
1:B:344:PHE:O	1:B:345:ALA:HB3	2.01	0.60
1:A:478:GLU:CB	1:A:482:LEU:HD22	2.32	0.60
1:A:141:SER:O	1:A:179:PRO:HB2	2.00	0.60
1:B:343:GLN:O	1:B:344:PHE:HB2	2.02	0.60
1:B:472:ARG:HH21	1:B:473:LEU:HD11	1.67	0.60
1:B:106:PHE:HB2	1:B:140:ASP:CG	2.23	0.59
1:B:104:GLN:CG	1:B:117:TYR:OH	2.50	0.59
1:A:266:PRO:HB2	1:A:333:PRO:HG2	1.83	0.59
1:A:366:PHE:O	1:A:367:ASN:HB2	2.01	0.59
1:B:269:PHE:O	1:B:269:PHE:HD2	1.82	0.59
1:A:11:ILE:HG23	1:A:12:HIS:N	2.16	0.59
1:A:520:LEU:HD21	1:B:165:HIS:NE2	2.18	0.59
1:B:451:VAL:O	1:B:455:HIS:HB2	2.02	0.59
1:A:254:LEU:CD2	1:A:312:PHE:HE2	2.15	0.59
1:A:415:LYS:HE3	1:A:417:PHE:HE2	1.67	0.59
1:A:457:ARG:NH1	1:A:457:ARG:HG3	2.18	0.59
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.84	0.58
1:B:299:HIS:HE1	1:B:313:GLU:OE2	1.86	0.58
1:B:358:ARG:HG2	4:B:567:HOH:O	2.02	0.58
1:A:169:VAL:HG12	1:A:170:ILE:HG23	1.86	0.58
1:A:215:THR:O	1:A:215:THR:CG2	2.51	0.58
1:B:65:ASP:OD2	1:B:123:LYS:HD2	2.03	0.58
1:B:87:VAL:CG1	1:B:117:TYR:CD2	2.86	0.58
1:A:211:ILE:HD12	1:A:211:ILE:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:HG3	1:A:386:GLU:O	2.02	0.58
1:A:477:TYR:CD1	1:A:482:LEU:HD11	2.37	0.58
1:B:200:THR:CG2	4:B:631:HOH:O	2.51	0.58
1:B:341:PRO:HB3	1:B:414:ARG:NH2	2.19	0.58
1:A:405:THR:HG22	1:A:518:GLU:O	2.03	0.57
1:A:457:ARG:HH11	1:A:457:ARG:HG3	1.69	0.57
1:A:86:GLY:C	1:A:117:TYR:CD2	2.78	0.57
1:A:181:ALA:HB1	1:A:204:PHE:CE1	2.38	0.57
1:B:126:ASP:OD1	1:B:162:ARG:HD3	2.04	0.57
1:A:10:ASP:C	1:A:16:GLY:HA3	2.25	0.57
1:B:173:ILE:HD12	1:B:255:LEU:HD21	1.87	0.57
1:B:124:VAL:HG12	1:B:125:MET:N	2.18	0.57
1:B:10:ASP:OD1	1:B:13:THR:HG23	2.05	0.57
1:A:503:ARG:O	1:A:503:ARG:HG2	2.05	0.57
1:B:478:GLU:O	1:B:482:LEU:HB2	2.05	0.57
1:B:113:LEU:HB3	1:B:156:TYR:CE1	2.40	0.57
1:B:214:VAL:HG12	1:B:215:THR:HG22	1.86	0.57
1:B:308:ASP:O	1:B:309:ALA:C	2.43	0.57
1:A:100:ALA:HB1	1:A:124:VAL:HG12	1.86	0.56
1:B:47:THR:OG1	1:B:50:GLU:HG3	2.04	0.56
1:B:113:LEU:CB	1:B:156:TYR:CE1	2.88	0.56
1:A:303:GLU:O	1:A:309:ALA:HA	2.04	0.56
1:A:315:GLN:HB2	1:A:355:LYS:HE3	1.88	0.56
1:A:477:TYR:O	1:A:482:LEU:CD1	2.53	0.56
1:A:405:THR:O	1:A:516:LYS:HE2	2.04	0.56
1:B:147:GLN:H	1:B:147:GLN:HE21	1.54	0.56
1:A:125:MET:HE1	1:A:163:ASN:ND2	2.20	0.56
1:B:98:PRO:C	1:B:99:VAL:HG23	2.24	0.56
1:A:462:ALA:C	1:A:464:ASP:N	2.58	0.56
1:A:149:GLY:C	1:B:444:VAL:HG23	2.25	0.56
1:A:503:ARG:O	1:A:507:VAL:CG2	2.52	0.56
1:A:390:ILE:HG23	1:A:391:ILE:N	2.21	0.56
1:A:433:LEU:HA	1:A:494:ASP:OD1	2.06	0.56
1:A:475:GLN:CD	1:A:475:GLN:O	2.45	0.56
1:B:163:ASN:HB3	1:B:190:ILE:CG2	2.34	0.55
1:A:477:TYR:O	1:A:482:LEU:HD13	2.07	0.55
1:A:340:GLN:CD	1:A:342:MET:HG3	2.26	0.55
1:A:462:ALA:C	1:A:464:ASP:H	2.10	0.55
1:B:462:ALA:C	1:B:464:ASP:H	2.09	0.55
1:B:271:GLU:O	1:B:271:GLU:HG3	2.07	0.55
1:B:339:ASN:ND2	1:B:424:MET:CE	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ILE:HG12	1:B:529:PRO:N	2.21	0.55
1:B:37:VAL:HG12	1:B:37:VAL:O	2.06	0.55
1:B:193:PHE:CD1	1:B:238:HIS:NE2	2.75	0.55
1:B:308:ASP:O	1:B:310:GLU:N	2.39	0.55
1:A:176:VAL:HB	1:A:196:MET:HG2	1.89	0.55
1:A:211:ILE:HD12	1:A:215:THR:HG22	1.88	0.55
1:A:464:ASP:O	1:A:465:ASP:HB2	2.05	0.55
1:A:390:ILE:HG13	1:B:186:TYR:OH	2.07	0.55
1:B:392:ARG:HG3	1:B:393:ARG:CG	2.26	0.55
1:B:417:PHE:CD1	1:B:443:ALA:HB3	2.42	0.55
1:A:54:LEU:HD21	1:A:245:LYS:HD2	1.89	0.55
1:A:113:LEU:HD23	1:A:156:TYR:CD2	2.43	0.55
1:B:13:THR:O	1:B:16:GLY:N	2.33	0.55
1:B:102:PHE:CE1	1:B:137:GLY:CA	2.90	0.55
1:B:503:ARG:O	1:B:507:VAL:HG23	2.06	0.55
1:B:24:ARG:O	1:B:67:PHE:HE1	1.90	0.54
1:B:158:GLU:CD	1:B:161:ARG:HH12	2.11	0.54
1:B:180:CYS:O	1:B:185:VAL:HG12	2.06	0.54
1:A:344:PHE:O	1:A:345:ALA:CB	2.54	0.54
1:A:350:ILE:O	1:A:354:GLU:HG3	2.07	0.54
1:A:70:HIS:HD2	1:A:72:SER:N	2.03	0.54
1:A:87:VAL:CB	1:A:117:TYR:HD2	2.17	0.54
1:B:61:PHE:HE2	1:B:63:GLU:HB2	1.70	0.54
1:B:501:ASP:O	1:B:505:HIS:HD2	1.89	0.54
1:A:379:PHE:HZ	1:A:423:VAL:HG21	1.72	0.54
1:A:409:ILE:CD1	1:A:510:LEU:HG	2.37	0.54
1:B:219:VAL:HG22	1:B:220:GLY:N	2.22	0.54
1:A:458:THR:O	1:A:458:THR:CG2	2.55	0.54
1:B:478:GLU:HA	1:B:482:LEU:HD13	1.88	0.54
1:A:458:THR:O	1:A:458:THR:HG22	2.08	0.54
1:A:520:LEU:HD22	1:B:165:HIS:CE1	2.42	0.54
1:B:467:GLU:OE1	1:B:467:GLU:N	2.30	0.54
1:A:52:ILE:HD11	1:A:88:VAL:HB	1.89	0.54
1:A:69:ARG:HD2	1:A:83:TYR:CE2	2.43	0.54
1:A:501:ASP:OD1	1:A:504:ARG:HB3	2.08	0.54
1:B:254:LEU:CD1	1:B:312:PHE:HE2	2.21	0.54
1:B:298:MET:O	1:B:302:ILE:HD12	2.08	0.54
1:A:219:VAL:HG22	1:A:223:GLU:HG2	1.90	0.53
1:A:160:PHE:CE1	1:A:187:SER:CB	2.84	0.53
1:A:181:ALA:HB2	1:A:204:PHE:CZ	2.43	0.53
1:B:94:VAL:O	1:B:95:ASP:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLU:HB3	1:B:162:ARG:HH12	1.73	0.53
1:B:403:GLU:HA	1:B:520:LEU:HD11	1.90	0.53
1:B:462:ALA:O	1:B:464:ASP:N	2.41	0.53
1:A:528:ILE:HG12	1:A:529:PRO:CD	2.38	0.53
1:A:113:LEU:HD13	1:A:117:TYR:CE1	2.43	0.53
1:A:387:HIS:O	1:A:388:ASP:C	2.45	0.53
1:A:102:PHE:CZ	1:A:137:GLY:HA3	2.44	0.53
1:A:219:VAL:CG2	1:A:223:GLU:HG2	2.38	0.53
1:A:379:PHE:CE1	1:A:420:ALA:HB2	2.43	0.53
1:A:528:ILE:CG1	1:A:529:PRO:HD2	2.38	0.53
1:A:178:GLY:O	1:A:201:SER:HA	2.09	0.53
1:A:254:LEU:HD23	1:A:312:PHE:CE2	2.42	0.53
1:B:87:VAL:CB	1:B:117:TYR:CE2	2.85	0.53
1:B:91:TYR:CD1	1:B:91:TYR:C	2.81	0.53
1:A:478:GLU:HG2	1:A:482:LEU:CD2	2.39	0.53
1:B:445:MET:HE3	1:B:449:GLY:CA	2.38	0.53
1:B:277:VAL:O	1:B:277:VAL:CG2	2.57	0.53
1:A:99:VAL:CG2	1:A:134:PRO:HB2	2.32	0.52
1:B:124:VAL:CG1	1:B:125:MET:N	2.71	0.52
1:B:433:LEU:HA	1:B:494:ASP:OD1	2.10	0.52
1:B:445:MET:CE	1:B:449:GLY:O	2.57	0.52
1:A:230:HIS:CE1	1:B:391:ILE:HD12	2.44	0.52
1:A:447:ALA:CB	1:A:478:GLU:HG2	2.40	0.52
1:A:63:GLU:HG2	1:A:66:GLU:HB2	1.91	0.52
1:B:33:SER:O	1:B:36:ALA:N	2.41	0.52
1:A:165:HIS:NE2	1:B:520:LEU:CD2	2.72	0.52
1:A:170:ILE:HG22	1:A:261:ASN:HB3	1.92	0.52
1:A:362:THR:HG22	1:A:366:PHE:CE2	2.45	0.52
1:B:528:ILE:CG1	1:B:529:PRO:CD	2.79	0.52
1:A:154:GLY:CA	1:B:428:HIS:CE1	2.91	0.52
1:A:188:PRO:O	1:A:191:THR:OG1	2.26	0.52
1:A:456:ARG:CZ	1:A:457:ARG:NH2	2.69	0.52
1:A:94:VAL:O	1:A:95:ASP:HB2	2.10	0.52
1:B:69:ARG:NH1	1:B:83:TYR:OH	2.43	0.52
1:B:180:CYS:O	1:B:185:VAL:CG1	2.57	0.52
1:A:234:SER:HA	1:B:387:HIS:O	2.10	0.52
1:A:482:LEU:CD1	1:A:482:LEU:N	2.73	0.52
1:A:275:LEU:CD2	1:A:507:VAL:HG21	2.40	0.51
1:A:438:PRO:HD3	1:A:497:ILE:O	2.10	0.51
1:B:11:ILE:CG2	1:B:12:HIS:N	2.72	0.51
1:A:125:MET:HE3	1:A:163:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:CD	1:A:148:GLU:OE2	2.56	0.51
1:B:111:GLY:O	1:B:141:SER:CB	2.59	0.51
1:B:314:THR:O	1:B:315:GLN:C	2.49	0.51
1:B:324:THR:HA	1:B:336:ILE:O	2.10	0.51
1:A:113:LEU:CD1	1:A:117:TYR:HD1	2.10	0.51
1:A:340:GLN:OE1	1:A:342:MET:HG3	2.11	0.51
1:A:381:PRO:HG2	1:B:214:VAL:HG11	1.92	0.51
1:B:326:PHE:CZ	1:B:359:PHE:CE1	2.98	0.51
1:A:70:HIS:HA	1:A:116:VAL:HG21	1.92	0.51
1:B:457:ARG:CG	1:B:457:ARG:NH1	2.38	0.51
1:A:134:PRO:HG3	1:A:171:PRO:HG2	1.91	0.51
1:B:160:PHE:CE1	1:B:187:SER:HB2	2.44	0.51
1:A:380:LEU:O	1:A:380:LEU:CD1	2.59	0.51
1:A:451:VAL:HG11	1:A:474:ILE:CA	2.37	0.50
1:A:455:HIS:O	1:A:459:ILE:CG2	2.58	0.50
1:B:401:TYR:CE2	1:B:423:VAL:O	2.64	0.50
1:B:40:GLN:HE22	1:B:45:LYS:NZ	2.10	0.50
1:A:299:HIS:O	1:A:303:GLU:HG3	2.11	0.50
1:A:444:VAL:HA	1:B:153:LEU:HD11	1.93	0.50
1:B:367:ASN:HA	1:B:406:VAL:HG11	1.92	0.50
1:A:211:ILE:HD12	1:A:215:THR:CG2	2.42	0.50
1:A:380:LEU:HD11	4:A:623:HOH:O	2.10	0.50
1:B:146:ILE:O	1:B:147:GLN:C	2.50	0.50
1:A:69:ARG:NH1	1:A:83:TYR:CZ	2.79	0.50
1:A:234:SER:HB2	1:A:236:VAL:HG23	1.94	0.50
1:B:91:TYR:CD1	1:B:91:TYR:O	2.65	0.50
1:A:176:VAL:HB	1:A:196:MET:CG	2.41	0.50
1:A:467:GLU:N	1:A:467:GLU:OE2	2.45	0.50
1:B:208:PRO:HD2	1:B:221:PHE:CZ	2.47	0.50
1:A:160:PHE:HE1	1:A:187:SER:CB	2.08	0.50
1:A:478:GLU:HA	1:A:482:LEU:CG	2.40	0.50
1:B:305:VAL:HG23	1:B:306:LEU:N	2.26	0.50
1:A:232:SER:O	1:A:318:PHE:HD1	1.95	0.49
1:A:475:GLN:O	1:A:475:GLN:OE1	2.30	0.49
1:B:111:GLY:O	1:B:141:SER:OG	2.23	0.49
1:A:406:VAL:O	1:A:408:LEU:HG	2.13	0.49
1:B:25:ILE:O	1:B:25:ILE:HG13	2.09	0.49
1:A:207:GLY:O	1:A:211:ILE:CG2	2.60	0.49
1:A:158:GLU:HB3	1:A:162:ARG:HH12	1.76	0.49
1:A:250:TYR:CE1	1:A:312:PHE:CZ	3.00	0.49
1:A:434:ASN:HB3	4:A:656:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ASP:CG	1:B:11:ILE:N	2.64	0.49
1:B:132:GLY:C	1:B:261:ASN:HD22	2.15	0.49
1:B:300:SER:O	1:B:304:HIS:ND1	2.40	0.49
1:A:80:ASN:N	1:A:80:ASN:ND2	2.61	0.49
1:A:121:ILE:O	1:A:125:MET:HG3	2.12	0.49
1:A:387:HIS:O	1:B:234:SER:HB2	2.12	0.49
1:A:483:ASN:CB	1:A:484:PRO:HD2	2.31	0.49
1:B:232:SER:O	1:B:318:PHE:HD1	1.95	0.49
1:B:435:LEU:HD13	1:B:435:LEU:N	2.27	0.49
1:B:445:MET:CE	1:B:449:GLY:CA	2.90	0.49
1:B:465:ASP:O	1:B:469:THR:HG23	2.12	0.49
1:A:113:LEU:CD1	1:A:117:TYR:CE1	2.95	0.49
1:A:175:LEU:C	1:A:175:LEU:CD2	2.81	0.49
1:A:324:THR:HA	1:A:336:ILE:O	2.13	0.49
1:B:226:GLY:O	1:B:229:THR:HB	2.13	0.49
1:B:329:VAL:O	1:B:330:GLU:HB2	2.12	0.49
1:A:265:GLU:CG	1:A:266:PRO:CD	2.90	0.49
1:B:36:ALA:HA	1:B:39:LYS:HG3	1.94	0.49
1:B:147:GLN:HE21	1:B:147:GLN:N	2.11	0.49
1:A:11:ILE:CG2	1:A:12:HIS:N	2.75	0.49
1:B:445:MET:CE	1:B:449:GLY:HA3	2.41	0.49
1:A:121:ILE:O	1:A:121:ILE:CG2	2.61	0.48
1:A:230:HIS:HE1	1:B:391:ILE:HD12	1.77	0.48
1:A:517:ARG:HD2	4:A:664:HOH:O	2.12	0.48
1:B:231:ASN:HD21	1:B:238:HIS:C	2.16	0.48
1:B:390:ILE:HG23	1:B:391:ILE:N	2.28	0.48
1:A:340:GLN:HG3	1:A:340:GLN:O	2.12	0.48
1:B:113:LEU:HA	1:B:117:TYR:CD1	2.48	0.48
1:B:483:ASN:HD22	1:B:483:ASN:C	2.17	0.48
1:A:349:ASP:O	1:A:350:ILE:C	2.52	0.48
1:B:473:LEU:HA	1:B:476:GLU:HG3	1.95	0.48
1:A:435:LEU:N	1:A:435:LEU:HD13	2.27	0.48
1:B:268:ALA:CB	1:B:332:ARG:HG3	2.43	0.48
1:B:437:TRP:NE1	1:B:502:THR:OG1	2.46	0.48
1:A:391:ILE:HA	1:B:186:TYR:CE1	2.48	0.48
1:B:113:LEU:HD13	1:B:156:TYR:CD1	2.41	0.48
1:B:208:PRO:CD	1:B:221:PHE:CE1	2.97	0.48
1:B:280:GLU:O	1:B:283:GLU:HB2	2.13	0.48
1:A:170:ILE:HG22	1:A:261:ASN:CB	2.43	0.48
1:A:392:ARG:HG3	1:A:393:ARG:N	2.28	0.48
1:A:409:ILE:HD11	1:A:510:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:O	1:B:37:VAL:CG1	2.61	0.48
1:A:193:PHE:HA	1:A:238:HIS:ND1	2.28	0.48
1:A:288:VAL:HG11	1:A:439:THR:HG21	1.95	0.48
1:A:459:ILE:HD11	1:A:466:ALA:O	2.14	0.48
1:B:61:PHE:CE2	1:B:63:GLU:HB2	2.48	0.48
1:B:253:GLN:O	1:B:256:SER:OG	2.22	0.48
1:B:455:HIS:CE1	1:B:473:LEU:HG	2.50	0.47
1:A:85:ASP:O	1:A:117:TYR:CB	2.57	0.47
1:A:147:GLN:HG3	1:B:454:LEU:CD2	2.43	0.47
1:A:159:ILE:HG22	1:A:163:ASN:OD1	2.14	0.47
1:B:23:ARG:NH2	1:B:24:ARG:HG3	2.29	0.47
1:B:187:SER:HB3	1:B:188:PRO:CD	2.35	0.47
1:B:188:PRO:O	1:B:191:THR:OG1	2.31	0.47
1:B:266:PRO:CG	1:B:368:VAL:HG22	2.44	0.47
1:B:320:PRO:HB2	1:B:343:GLN:HG3	1.96	0.47
1:A:134:PRO:HG3	1:A:171:PRO:CG	2.45	0.47
1:A:56:LEU:HD11	1:A:101:VAL:HG11	1.96	0.47
1:B:132:GLY:HA3	1:B:261:ASN:ND2	2.29	0.47
1:B:173:ILE:HD12	1:B:255:LEU:CD2	2.43	0.47
1:A:113:LEU:HD13	1:A:117:TYR:HE1	1.78	0.47
1:A:170:ILE:HG13	1:A:170:ILE:O	2.15	0.47
1:A:306:LEU:HD21	1:A:336:ILE:HD11	1.96	0.47
1:A:389:GLY:O	1:A:393:ARG:HG3	2.13	0.47
1:A:451:VAL:HG23	1:A:452:ASN:N	2.29	0.47
1:A:478:GLU:HG2	1:A:482:LEU:HD22	1.97	0.47
1:A:483:ASN:C	1:A:483:ASN:HD22	2.17	0.47
1:B:318:PHE:O	1:B:355:LYS:HD2	2.15	0.47
1:B:472:ARG:HE	1:B:473:LEU:HD13	1.79	0.47
1:B:287:ILE:HG12	1:B:296:TYR:CD2	2.50	0.47
1:B:474:ILE:O	1:B:478:GLU:OE1	2.32	0.47
1:A:48:ALA:O	1:A:52:ILE:HG13	2.14	0.47
1:B:23:ARG:NE	1:B:23:ARG:C	2.68	0.47
1:B:322:ILE:CG2	1:B:355:LYS:HD3	2.45	0.47
1:A:13:THR:O	1:A:16:GLY:N	2.48	0.46
1:A:193:PHE:CE2	1:A:362:THR:HG21	2.50	0.46
1:B:170:ILE:O	1:B:170:ILE:HG13	2.15	0.46
1:A:10:ASP:N	1:A:13:THR:HG23	2.29	0.46
1:A:186:TYR:OH	1:B:390:ILE:HG13	2.14	0.46
1:A:227:ALA:HB3	4:A:571:HOH:O	2.14	0.46
1:A:350:ILE:HG13	1:A:385:GLN:NE2	2.30	0.46
1:A:390:ILE:CG1	1:B:186:TYR:OH	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:MET:O	1:A:499:PRO:C	2.54	0.46
1:B:25:ILE:CD1	4:B:644:HOH:O	2.45	0.46
1:B:401:TYR:CE2	1:B:425:GLY:N	2.83	0.46
1:A:503:ARG:O	1:A:503:ARG:CG	2.63	0.46
1:B:204:PHE:CE1	1:B:207:GLY:HA2	2.51	0.46
1:B:221:PHE:CB	2:B:5601:BTN:H81	2.45	0.46
1:B:284:LEU:HD21	1:B:304:HIS:CG	2.51	0.46
1:A:284:LEU:HG	1:A:304:HIS:CD2	2.50	0.46
1:A:386:GLU:OE2	1:B:204:PHE:CA	2.63	0.46
1:A:389:GLY:O	1:A:393:ARG:CG	2.64	0.46
1:B:221:PHE:HB2	2:B:5601:BTN:H81	1.97	0.46
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.75	0.46
1:B:395:ALA:O	1:B:398:ILE:HG23	2.15	0.46
1:A:87:VAL:N	1:A:117:TYR:HD2	2.13	0.46
1:A:302:ILE:O	1:A:305:VAL:CG2	2.61	0.46
1:B:81:ARG:N	1:B:82:PRO:HD3	2.29	0.46
1:B:376:VAL:O	1:B:376:VAL:HG13	2.15	0.46
1:A:102:PHE:CE1	1:A:137:GLY:HA3	2.51	0.46
1:B:70:HIS:CD2	1:B:70:HIS:C	2.88	0.46
1:B:193:PHE:HA	1:B:238:HIS:ND1	2.26	0.46
1:B:457:ARG:O	1:B:460:ALA:N	2.48	0.46
1:A:128:ALA:HB1	1:A:133:CYS:O	2.16	0.46
1:A:469:THR:O	1:A:472:ARG:CB	2.61	0.46
1:A:522:PRO:O	1:A:523:LYS:HB3	2.16	0.46
1:A:398:ILE:HD11	1:B:160:PHE:HB3	1.93	0.46
1:A:520:LEU:HD22	1:B:165:HIS:CG	2.50	0.46
1:B:128:ALA:CB	1:B:135:VAL:CG2	2.93	0.46
1:A:454:LEU:HD13	1:B:75:PHE:CZ	2.51	0.46
1:B:116:VAL:O	1:B:120:LYS:N	2.46	0.46
1:A:198:ASP:CG	1:A:199:GLN:HG2	2.36	0.45
1:A:361:ARG:NH2	4:A:532:HOH:O	2.38	0.45
1:A:498:MET:O	1:A:500:SER:N	2.49	0.45
1:B:187:SER:H	1:B:188:PRO:HD2	1.81	0.45
1:B:198:ASP:OD1	1:B:199:GLN:N	2.49	0.45
1:B:456:ARG:O	1:B:459:ILE:HG22	2.14	0.45
1:A:183:GLY:O	1:A:184:ALA:C	2.54	0.45
1:A:284:LEU:HD21	1:A:304:HIS:CG	2.51	0.45
1:A:528:ILE:HG12	1:A:529:PRO:N	2.31	0.45
1:B:266:PRO:HG3	1:B:368:VAL:HG22	1.99	0.45
1:B:69:ARG:NH1	1:B:83:TYR:CZ	2.84	0.45
1:B:341:PRO:HB3	1:B:414:ARG:HH22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:CB	1:B:454:LEU:HD11	2.44	0.45
1:A:165:HIS:CD2	1:B:520:LEU:CD2	2.96	0.45
1:A:196:MET:HE3	1:A:203:MET:HG3	1.99	0.45
1:A:256:SER:O	1:A:267:PRO:HG2	2.17	0.45
1:A:493:VAL:HG23	1:A:493:VAL:O	2.17	0.45
1:B:467:GLU:H	1:B:467:GLU:CD	2.17	0.45
1:A:26:GLU:O	1:A:30:HIS:HD2	1.99	0.45
1:A:113:LEU:CD2	1:A:156:TYR:CD1	2.99	0.45
1:A:322:ILE:HG13	1:A:338:ALA:O	2.16	0.45
1:B:87:VAL:HB	1:B:117:TYR:HE2	1.74	0.45
1:B:401:TYR:CZ	1:B:425:GLY:N	2.85	0.45
1:A:102:PHE:CZ	1:A:137:GLY:CA	2.99	0.45
1:A:486:THR:HB	4:A:565:HOH:O	2.16	0.45
1:B:195:VAL:CG2	1:B:247:ALA:HB1	2.47	0.45
1:B:456:ARG:HE	1:B:456:ARG:HB2	1.42	0.45
1:A:91:TYR:CD1	1:A:91:TYR:C	2.89	0.45
1:B:56:LEU:CD1	1:B:61:PHE:HD1	2.30	0.45
1:A:99:VAL:HG22	1:A:134:PRO:CB	2.32	0.45
1:B:13:THR:O	1:B:14:THR:C	2.55	0.45
1:B:72:SER:O	1:B:78:ASP:HB3	2.16	0.45
1:B:158:GLU:O	1:B:162:ARG:NH1	2.47	0.45
1:B:474:ILE:O	1:B:478:GLU:HG3	2.17	0.45
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.99	0.45
1:A:327:GLY:O	1:A:328:ARG:HG2	2.17	0.45
1:A:436:ALA:O	1:A:496:VAL:HA	2.16	0.45
1:B:128:ALA:HB2	1:B:135:VAL:CG2	2.46	0.45
1:B:483:ASN:HB2	1:B:484:PRO:HD2	1.98	0.45
1:B:349:ASP:O	1:B:350:ILE:C	2.55	0.45
1:B:456:ARG:C	1:B:459:ILE:HG22	2.37	0.45
1:A:60:SER:O	1:A:61:PHE:C	2.55	0.44
1:A:262:ASN:OD1	1:A:262:ASN:O	2.36	0.44
1:A:389:GLY:O	1:A:393:ARG:HD3	2.16	0.44
1:B:321:ASN:OD1	1:B:321:ASN:N	2.47	0.44
1:B:399:PHE:O	1:B:399:PHE:CD2	2.69	0.44
1:A:156:TYR:HB3	1:A:160:PHE:CE2	2.52	0.44
1:B:198:ASP:CG	1:B:199:GLN:HG2	2.35	0.44
1:A:161:ARG:NH2	1:A:162:ARG:NH2	2.65	0.44
1:A:478:GLU:HB3	1:A:482:LEU:HD22	1.98	0.44
1:B:40:GLN:HE22	1:B:45:LYS:HZ1	1.63	0.44
1:B:363:CYS:HB3	1:B:368:VAL:HB	1.98	0.44
1:A:86:GLY:O	1:A:117:TYR:HE2	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:O	1:A:145:ARG:CB	2.57	0.44
1:A:329:VAL:O	1:A:330:GLU:CB	2.64	0.44
1:B:187:SER:N	1:B:188:PRO:CD	2.80	0.44
1:A:288:VAL:HG22	1:A:296:TYR:CZ	2.53	0.44
1:A:196:MET:CE	1:A:230:HIS:HD2	2.31	0.44
1:B:70:HIS:HD2	1:B:72:SER:N	2.16	0.44
1:B:427:LYS:HB2	1:B:427:LYS:HE2	1.73	0.44
1:A:215:THR:CG2	1:A:217:GLU:HB3	2.47	0.44
1:A:376:VAL:O	1:A:376:VAL:CG1	2.64	0.44
1:A:380:LEU:C	1:A:380:LEU:CD1	2.77	0.44
1:A:433:LEU:HD12	1:A:494:ASP:OD1	2.18	0.44
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.35	0.44
1:B:198:ASP:HA	1:B:227:ALA:HB3	2.00	0.44
1:B:493:VAL:HG23	1:B:493:VAL:O	2.16	0.44
1:A:158:GLU:CD	1:A:161:ARG:HH12	2.21	0.44
1:A:182:GLY:O	1:A:185:VAL:HG22	2.18	0.44
1:A:448:GLN:O	1:A:452:ASN:OD1	2.36	0.44
1:B:466:ALA:O	1:B:467:GLU:C	2.56	0.44
1:B:469:THR:O	1:B:473:LEU:HD22	2.18	0.44
1:B:473:LEU:HA	1:B:473:LEU:HD12	1.80	0.44
1:A:21:LEU:O	1:A:21:LEU:CG	2.65	0.43
1:A:102:PHE:CE1	1:A:137:GLY:CA	3.01	0.43
1:A:456:ARG:HD2	1:A:457:ARG:CZ	2.48	0.43
1:A:478:GLU:CG	1:A:482:LEU:HD22	2.47	0.43
1:B:130:LYS:HE3	1:B:130:LYS:HB2	1.67	0.43
1:B:204:PHE:CZ	1:B:221:PHE:HE1	2.36	0.43
1:B:208:PRO:HD2	1:B:221:PHE:CE1	2.52	0.43
1:B:364:ASP:CG	1:B:404:ALA:HA	2.38	0.43
1:A:212:LYS:CE	1:A:218:ASP:OD1	2.67	0.43
1:B:182:GLY:O	1:B:185:VAL:HG22	2.18	0.43
1:B:326:PHE:CE2	1:B:359:PHE:HE1	2.35	0.43
1:B:434:ASN:C	1:B:435:LEU:HD13	2.38	0.43
1:A:395:ALA:C	1:A:398:ILE:HG23	2.33	0.43
1:A:475:GLN:O	1:A:475:GLN:CG	2.66	0.43
1:B:344:PHE:O	1:B:345:ALA:CB	2.66	0.43
1:B:455:HIS:O	1:B:456:ARG:C	2.56	0.43
1:A:475:GLN:CD	1:A:475:GLN:C	2.77	0.43
1:B:284:LEU:HG	1:B:304:HIS:CD2	2.53	0.43
1:B:205:ILE:H	1:B:205:ILE:HG13	1.30	0.43
1:B:478:GLU:HG2	1:B:482:LEU:HD22	1.99	0.43
1:A:433:LEU:HA	1:A:433:LEU:HD12	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLU:HA	1:A:482:LEU:CD2	2.49	0.43
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.83	0.43
1:A:445:MET:SD	1:A:449:GLY:O	2.77	0.43
1:B:77:LEU:HD21	1:B:109:PHE:CZ	2.54	0.43
1:B:219:VAL:HG22	1:B:220:GLY:O	2.18	0.43
1:A:11:ILE:C	1:A:13:THR:H	2.21	0.43
1:A:160:PHE:HB3	1:B:398:ILE:CD1	2.43	0.43
1:A:212:LYS:O	1:A:216:GLY:N	2.46	0.43
1:A:250:TYR:CZ	1:A:312:PHE:CZ	3.07	0.43
1:B:200:THR:HG21	4:B:631:HOH:O	2.17	0.43
1:A:478:GLU:HA	1:A:482:LEU:HD22	1.99	0.43
1:B:364:ASP:OD1	1:B:405:THR:N	2.48	0.43
1:B:419:GLY:O	1:B:423:VAL:HG23	2.19	0.43
1:B:457:ARG:C	1:B:459:ILE:N	2.71	0.43
1:A:337:VAL:O	1:A:372:THR:HA	2.18	0.43
1:A:343:GLN:O	1:A:344:PHE:HB2	2.19	0.43
1:A:409:ILE:HD12	1:A:510:LEU:HG	2.00	0.43
1:A:504:ARG:CG	1:A:508:ARG:HD2	2.45	0.43
1:B:40:GLN:NE2	1:B:45:LYS:NZ	2.66	0.43
1:B:266:PRO:CD	1:B:367:ASN:O	2.67	0.43
1:B:472:ARG:O	1:B:476:GLU:HG3	2.19	0.43
1:A:10:ASP:O	1:A:10:ASP:CG	2.57	0.42
1:A:187:SER:CB	1:A:188:PRO:HD3	2.21	0.42
1:A:148:GLU:O	1:A:151:ALA:HB3	2.20	0.42
1:A:175:LEU:CD2	1:A:177:VAL:HG13	2.42	0.42
1:B:85:ASP:O	1:B:117:TYR:HD2	2.02	0.42
1:A:493:VAL:O	1:A:494:ASP:C	2.58	0.42
1:A:520:LEU:CD2	1:B:165:HIS:CD2	2.94	0.42
1:B:20:ASP:HB3	4:B:539:HOH:O	2.19	0.42
1:B:315:GLN:HB2	1:B:355:LYS:HE3	2.01	0.42
1:A:86:GLY:C	1:A:117:TYR:HD2	2.22	0.42
1:B:332:ARG:NH2	1:B:514:ARG:HH12	2.17	0.42
1:A:387:HIS:O	1:B:234:SER:HA	2.19	0.42
1:B:198:ASP:O	1:B:199:GLN:HB2	2.19	0.42
1:A:466:ALA:O	1:A:469:THR:OG1	2.33	0.42
1:B:169:VAL:HG12	1:B:170:ILE:HG23	2.02	0.42
1:B:399:PHE:CG	1:B:528:ILE:HG13	2.54	0.42
1:A:192:ASP:O	1:A:238:HIS:CE1	2.72	0.42
1:B:146:ILE:HG23	1:B:147:GLN:N	2.34	0.42
1:B:390:ILE:O	1:B:394:GLY:N	2.43	0.42
1:A:146:ILE:HG21	1:B:454:LEU:CD1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:O	1:A:156:TYR:CD2	2.72	0.42
1:A:262:ASN:OD1	1:A:262:ASN:C	2.58	0.42
1:A:87:VAL:HG21	1:A:121:ILE:HD11	2.01	0.42
1:A:459:ILE:HG13	1:A:459:ILE:O	2.20	0.42
1:A:483:ASN:HD22	1:A:483:ASN:N	2.18	0.42
1:B:234:SER:O	1:B:236:VAL:N	2.53	0.42
1:B:341:PRO:HG3	1:B:375:ASP:OD2	2.19	0.42
1:B:364:ASP:OD1	1:B:404:ALA:HA	2.19	0.42
1:B:521:PRO:HA	1:B:522:PRO:HD3	1.93	0.42
1:A:161:ARG:HB2	1:B:429:LEU:HD23	2.01	0.42
1:A:451:VAL:CG2	1:A:474:ILE:HG12	2.37	0.42
1:B:113:LEU:CG	1:B:117:TYR:CE1	3.02	0.42
1:A:279:ASP:O	1:A:283:GLU:HG3	2.20	0.41
1:B:22:ARG:HA	1:B:25:ILE:HG23	1.99	0.41
1:B:98:PRO:C	1:B:99:VAL:CG2	2.87	0.41
1:A:196:MET:SD	1:A:203:MET:CE	2.98	0.41
1:B:363:CYS:O	1:B:368:VAL:O	2.38	0.41
1:A:113:LEU:HD23	1:A:156:TYR:CE1	2.43	0.41
1:A:513:LEU:C	1:A:515:THR:H	2.23	0.41
1:B:128:ALA:HB1	1:B:170:ILE:HD12	2.03	0.41
1:A:40:GLN:HE22	1:A:45:LYS:NZ	2.18	0.41
1:A:387:HIS:O	1:A:389:GLY:N	2.54	0.41
1:B:339:ASN:OD1	1:B:424:MET:CE	2.68	0.41
1:B:523:LYS:HE2	1:B:523:LYS:HB3	1.87	0.41
1:B:457:ARG:C	1:B:459:ILE:H	2.22	0.41
1:B:435:LEU:N	1:B:435:LEU:CD1	2.83	0.41
1:A:358:ARG:CG	1:A:358:ARG:O	2.68	0.41
1:A:403:GLU:HA	1:A:520:LEU:CD1	2.49	0.41
1:B:133:CYS:HA	1:B:134:PRO:HD3	1.74	0.41
1:B:302:ILE:O	1:B:305:VAL:CG2	2.60	0.41
1:A:478:GLU:HG2	1:A:482:LEU:HD21	2.02	0.41
1:B:80:ASN:O	1:B:82:PRO:HD3	2.20	0.41
1:B:318:PHE:O	1:B:319:ALA:HB3	2.20	0.41
1:A:69:ARG:NH1	1:A:83:TYR:OH	2.54	0.41
1:A:134:PRO:CB	1:A:171:PRO:HG2	2.51	0.41
1:A:154:GLY:HA2	1:B:428:HIS:NE2	2.36	0.41
1:A:211:ILE:O	1:A:215:THR:HG22	2.20	0.41
1:A:248:VAL:HG12	1:A:252:LYS:HD2	2.02	0.41
1:A:256:SER:HA	4:A:666:HOH:O	2.19	0.41
1:A:325:GLY:O	1:A:359:PHE:HZ	2.04	0.41
1:A:380:LEU:HD13	1:A:381:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LEU:C	1:A:515:THR:N	2.71	0.41
1:B:47:THR:O	1:B:51:ARG:HD2	2.20	0.41
1:B:100:ALA:O	1:B:135:VAL:HA	2.21	0.41
1:B:192:ASP:O	1:B:238:HIS:CE1	2.74	0.41
1:B:195:VAL:HG11	1:B:251:VAL:HG22	2.03	0.41
1:A:366:PHE:O	1:A:367:ASN:CB	2.65	0.41
1:A:414:ARG:O	1:A:441:GLN:N	2.43	0.41
1:B:102:PHE:CE1	1:B:137:GLY:HA2	2.55	0.41
1:B:183:GLY:O	1:B:184:ALA:C	2.60	0.41
1:B:231:ASN:ND2	1:B:238:HIS:C	2.74	0.41
1:B:417:PHE:CZ	1:B:441:GLN:HB2	2.56	0.41
1:B:437:TRP:HE1	1:B:502:THR:HG1	1.67	0.41
1:B:451:VAL:HB	1:B:455:HIS:CD2	2.45	0.41
1:A:406:VAL:HB	1:A:407:PRO:HD2	2.03	0.40
1:A:11:ILE:O	1:A:17:LYS:HG3	2.21	0.40
1:A:203:MET:O	1:A:225:GLY:HA3	2.21	0.40
1:A:284:LEU:CD2	1:A:304:HIS:CD2	3.05	0.40
1:A:512:GLN:O	1:A:513:LEU:C	2.58	0.40
1:B:166:ALA:O	1:B:169:VAL:N	2.47	0.40
1:A:377:PRO:HA	1:A:417:PHE:HD2	1.85	0.40
1:B:266:PRO:HD3	1:B:367:ASN:O	2.21	0.40
1:B:287:ILE:CG2	1:B:288:VAL:H	2.32	0.40
1:B:340:GLN:O	1:B:340:GLN:HG3	2.20	0.40
1:B:430:GLY:O	4:B:581:HOH:O	2.21	0.40
1:B:504:ARG:HH11	1:B:508:ARG:HH11	1.69	0.40
1:B:98:PRO:O	1:B:99:VAL:HG22	2.19	0.40
1:A:70:HIS:CE1	1:A:77:LEU:O	2.74	0.40
1:A:175:LEU:HD22	1:A:175:LEU:C	2.42	0.40
1:A:287:ILE:O	1:A:287:ILE:CG1	2.58	0.40
1:B:20:ASP:OD1	1:B:23:ARG:NH2	2.54	0.40
1:B:483:ASN:HD22	1:B:483:ASN:N	2.18	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	519/530 (98%)	459 (88%)	58 (11%)	2 (0%)	34 30
1	B	519/530 (98%)	458 (88%)	60 (12%)	1 (0%)	47 44
All	All	1038/1060 (98%)	917 (88%)	118 (11%)	3 (0%)	41 37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	GLY
1	A	514	ARG
1	B	98	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	412/421 (98%)	374 (91%)	38 (9%)	9 5
1	B	412/421 (98%)	375 (91%)	37 (9%)	9 6
All	All	824/842 (98%)	749 (91%)	75 (9%)	9 5

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	35	ARG
1	A	40	GLN
1	A	43	LYS
1	A	53	ASP
1	A	80	ASN
1	A	117	TYR
1	A	119	GLN
1	A	129	LEU
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	175	LEU
1	A	205	ILE
1	A	209	ASP
1	A	211	ILE
1	A	213	THR
1	A	215	THR
1	A	219	VAL
1	A	223	GLU
1	A	232	SER
1	A	245	LYS
1	A	263	LEU
1	A	264	SER
1	A	271	GLU
1	A	275	LEU
1	A	287	ILE
1	A	291	SER
1	A	342	MET
1	A	398	ILE
1	A	433	LEU
1	A	435	LEU
1	A	444	VAL
1	A	457	ARG
1	A	461	ASP
1	A	475	GLN
1	A	483	ASN
1	A	500	SER
1	A	527	ASN
1	A	528	ILE
1	B	23	ARG
1	B	25	ILE
1	B	35	ARG
1	B	39	LYS
1	B	40	GLN
1	B	49	ARG
1	B	77	LEU
1	B	124	VAL
1	B	146	ILE
1	B	147	GLN
1	B	177	VAL
1	B	195	VAL
1	B	200	THR
1	B	205	ILE

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Mol	Chain	Res	Type
1	B	212	LYS
1	B	213	THR
1	B	218	ASP
1	B	232	SER
1	B	245	LYS
1	B	254	LEU
1	B	280	GLU
1	B	293	ASN
1	B	342	MET
1	B	349	ASP
1	B	358	ARG
1	B	387	HIS
1	B	398	ILE
1	B	435	LEU
1	B	451	VAL
1	B	456	ARG
1	B	457	ARG
1	B	458	THR
1	B	461	ASP
1	B	472	ARG
1	B	473	LEU
1	B	483	ASN
1	B	508	ARG

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

Mol	Chain	Res	Type
1	A	30	HIS
1	A	40	GLN
1	A	70	HIS
1	A	74	ASN
1	A	80	ASN
1	A	119	GLN
1	A	147	GLN
1	A	230	HIS
1	A	231	ASN
1	A	299	HIS
1	A	385	GLN
1	A	448	GLN
1	A	455	HIS
1	A	483	ASN
1	A	505	HIS

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Mol	Chain	Res	Type
1	A	512	GLN
1	A	527	ASN
1	B	30	HIS
1	B	40	GLN
1	B	70	HIS
1	B	74	ASN
1	B	147	GLN
1	B	231	ASN
1	B	293	ASN
1	B	299	HIS
1	B	455	HIS
1	B	483	ASN
1	B	505	HIS
1	B	527	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	BTN	B	5601	-	14,17,17	3.82	7 (50%)	19,23,23	3.86	8 (42%)
3	SO4	A	531	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	B	531	-	4,4,4	0.22	0	6,6,6	0.11	0
2	BTN	A	5600	-	14,17,17	4.19	7 (50%)	19,23,23	3.65	8 (42%)

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	BTN	B	5601	-	-	2/5/28/28	0/2/2/2
2	BTN	A	5600	-	-	2/5/28/28	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5600	BTN	C5-N1	8.03	1.58	1.46
2	B	5601	BTN	C5-N1	6.78	1.56	1.46
2	A	5600	BTN	C2-S1	6.77	1.93	1.82
2	A	5600	BTN	C3-N2	6.67	1.46	1.35
2	B	5601	BTN	C2-S1	6.59	1.93	1.82
2	B	5601	BTN	C3-N2	5.88	1.45	1.35
2	A	5600	BTN	C4-N2	5.80	1.56	1.45
2	B	5601	BTN	C4-N2	5.37	1.55	1.45
2	A	5600	BTN	C3-N1	-4.97	1.27	1.35
2	B	5601	BTN	C3-N1	-4.80	1.27	1.35
2	A	5600	BTN	C6-S1	3.90	1.92	1.81
2	B	5601	BTN	C6-S1	3.78	1.92	1.81
2	A	5600	BTN	O3-C3	3.31	1.30	1.23
2	B	5601	BTN	O3-C3	2.70	1.29	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5601	BTN	C4-N2-C3	-8.12	105.05	112.62
2	A	5600	BTN	C4-N2-C3	-7.75	105.39	112.62
2	B	5601	BTN	O3-C3-N2	-7.72	114.86	125.94
2	B	5601	BTN	C6-C5-C4	7.46	115.14	108.66
2	A	5600	BTN	C6-C5-C4	7.34	115.03	108.66
2	A	5600	BTN	O3-C3-N2	-6.73	116.28	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5600	BTN	C6-C5-N1	-5.45	106.10	113.03
2	B	5601	BTN	C6-C5-N1	-5.38	106.19	113.03
2	B	5601	BTN	N2-C3-N1	5.37	113.80	108.76
2	A	5600	BTN	N2-C3-N1	4.66	113.13	108.76
2	A	5600	BTN	C5-C4-N2	3.78	106.74	102.67
2	B	5601	BTN	O3-C3-N1	3.76	131.34	125.94
2	B	5601	BTN	C5-C4-N2	3.69	106.64	102.67
2	A	5600	BTN	O3-C3-N1	3.24	130.59	125.94
2	B	5601	BTN	C5-C6-S1	-2.51	104.15	106.31
2	A	5600	BTN	C2-C4-N2	2.05	114.96	113.13

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5600	BTN	C11-C10-C9-C8
2	B	5601	BTN	C11-C10-C9-C8
2	A	5600	BTN	C7-C8-C9-C10
2	B	5601	BTN	C7-C8-C9-C10

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5601	BTN	2	0
2	A	5600	BTN	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.