Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2023 – 08:55 pm GMT

PDB ID	:	6QXA
Title	:	Structure of membrane bound pyrophosphatase from Thermotoga maritima in complex with imidodiphosphate and N-[(2-amino-6-benzothiazolyl)methyl]-1 H-indole-2-carboxamide (ATC)
Authors	:	Vidilaseris, K.; Goldman, A.
Deposited on	:	2019-03-07
Resolution	:	3.41 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 ⓘ symbol.

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

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

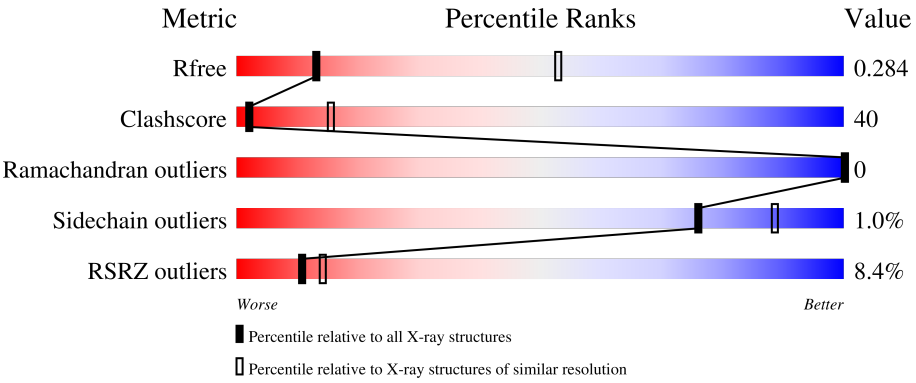
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	735	6% 43% 55%
1	B	735	11% 40% 57%
1	C	735	7% 43% 55%
1	D	735	9% 44% 53%

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
6	GQB	C	808	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 21095 atoms, of which 53 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 K(+)-stimulated pyrophosphate-energized sodium pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5260	3444	827	962	27			
1	B	715	Total	C	N	O	S	0	0	0
			5179	3397	810	946	26			
1	C	725	Total	C	N	O	S	0	0	0
			5267	3447	830	963	27			
1	D	719	Total	C	N	O	S	0	0	0
			5189	3407	804	951	27			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9S5X0
A	-7	ARG	-	expression tag	UNP Q9S5X0
A	-6	GLY	-	expression tag	UNP Q9S5X0
A	-5	SER	-	expression tag	UNP Q9S5X0
A	-4	HIS	-	expression tag	UNP Q9S5X0
A	-3	HIS	-	expression tag	UNP Q9S5X0
A	-2	HIS	-	expression tag	UNP Q9S5X0
A	-1	HIS	-	expression tag	UNP Q9S5X0
A	0	HIS	-	expression tag	UNP Q9S5X0
A	1	HIS	-	expression tag	UNP Q9S5X0
A	353	LEU	VAL	conflict	UNP Q9S5X0
A	395	GLY	SER	conflict	UNP Q9S5X0
B	-8	MET	-	initiating methionine	UNP Q9S5X0
B	-7	ARG	-	expression tag	UNP Q9S5X0
B	-6	GLY	-	expression tag	UNP Q9S5X0
B	-5	SER	-	expression tag	UNP Q9S5X0
B	-4	HIS	-	expression tag	UNP Q9S5X0
B	-3	HIS	-	expression tag	UNP Q9S5X0
B	-2	HIS	-	expression tag	UNP Q9S5X0
B	-1	HIS	-	expression tag	UNP Q9S5X0
B	0	HIS	-	expression tag	UNP Q9S5X0

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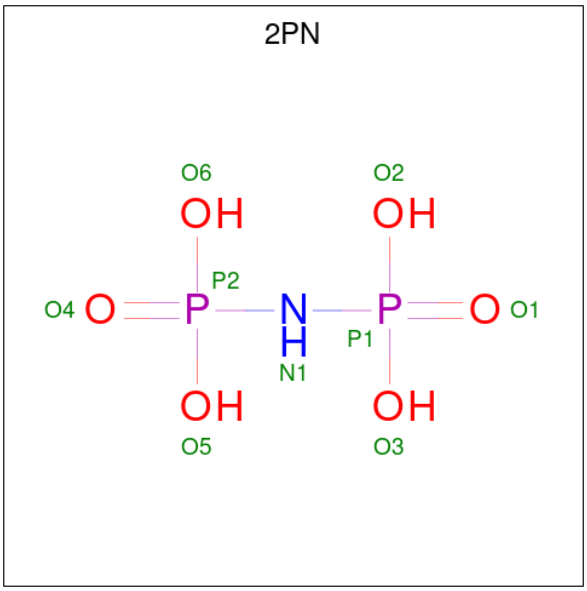
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	HIS	-	expression tag	UNP Q9S5X0
B	353	LEU	VAL	conflict	UNP Q9S5X0
B	395	GLY	SER	conflict	UNP Q9S5X0
C	-8	MET	-	initiating methionine	UNP Q9S5X0
C	-7	ARG	-	expression tag	UNP Q9S5X0
C	-6	GLY	-	expression tag	UNP Q9S5X0
C	-5	SER	-	expression tag	UNP Q9S5X0
C	-4	HIS	-	expression tag	UNP Q9S5X0
C	-3	HIS	-	expression tag	UNP Q9S5X0
C	-2	HIS	-	expression tag	UNP Q9S5X0
C	-1	HIS	-	expression tag	UNP Q9S5X0
C	0	HIS	-	expression tag	UNP Q9S5X0
C	1	HIS	-	expression tag	UNP Q9S5X0
C	353	LEU	VAL	conflict	UNP Q9S5X0
C	395	GLY	SER	conflict	UNP Q9S5X0
D	-8	MET	-	initiating methionine	UNP Q9S5X0
D	-7	ARG	-	expression tag	UNP Q9S5X0
D	-6	GLY	-	expression tag	UNP Q9S5X0
D	-5	SER	-	expression tag	UNP Q9S5X0
D	-4	HIS	-	expression tag	UNP Q9S5X0
D	-3	HIS	-	expression tag	UNP Q9S5X0
D	-2	HIS	-	expression tag	UNP Q9S5X0
D	-1	HIS	-	expression tag	UNP Q9S5X0
D	0	HIS	-	expression tag	UNP Q9S5X0
D	1	HIS	-	expression tag	UNP Q9S5X0
D	353	LEU	VAL	conflict	UNP Q9S5X0
D	395	GLY	SER	conflict	UNP Q9S5X0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0
2	B	5	Total Mg 5 5	0	0
2	C	5	Total Mg 5 5	0	0
2	D	5	Total Mg 5 5	0	0

- Molecule 3 is IMIDODIPHOSPHORIC ACID (three-letter code: 2PN) (formula: $H_5NO_6P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O P 9 1 6 2	0	0
3	B	1	Total N O P 9 1 6 2	0	0
3	C	1	Total N O P 9 1 6 2	0	0
3	D	1	Total N O P 9 1 6 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0

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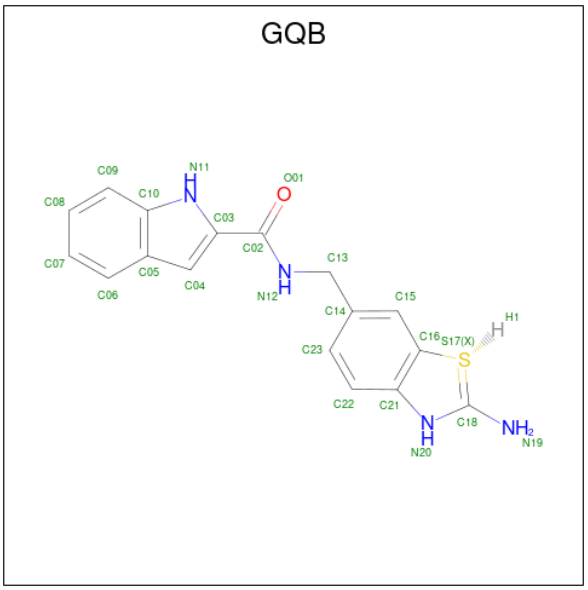
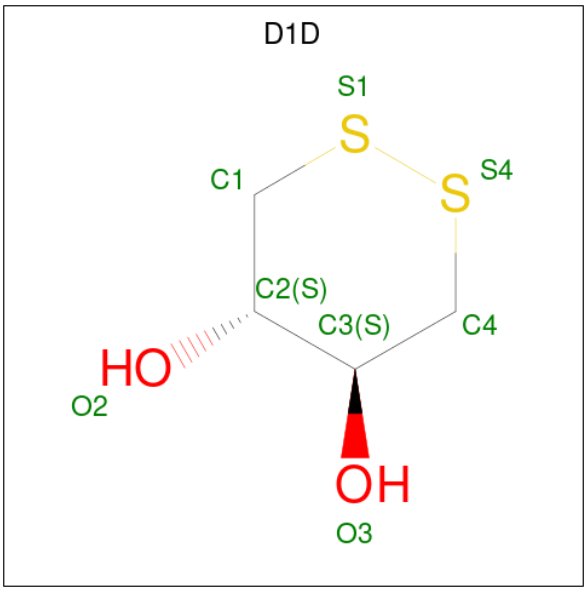
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0

- Molecule 6 is {N}-[(2-azanyl-3 {H}-1,3-benzothiazol-6-yl)methyl]-1 {H}-indole-2-carboxamide (three-letter code: GQB) (formula: $C_{17}H_{16}N_4OS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H N O S 38 17 15 4 1 1	0	0
6	A	1	Total C H N O S 38 17 15 4 1 1	0	0
6	C	1	Total C H N O S 38 17 15 4 1 1	0	0

- Molecule 7 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (three-letter code: D1D) (formula: $C_4H_8O_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	H	O	S	0	0
			16	4	8	2	2		

- Molecule 8 is water.

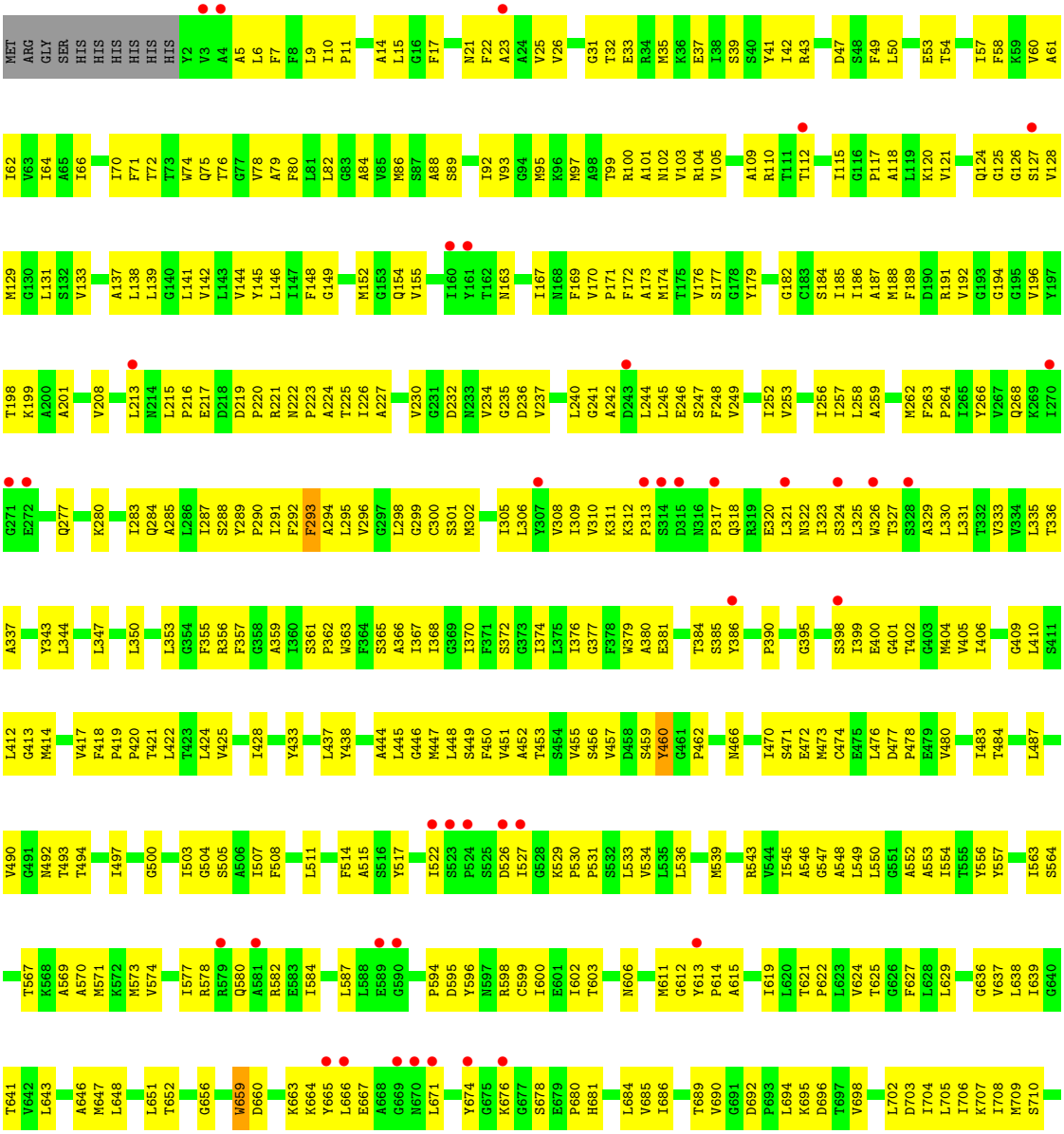
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		
8	C	3	Total	O	0	0
			3	3		
8	D	4	Total	O	0	0
			4	4		

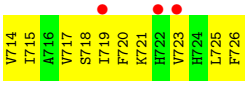
3 Residue-property plots (i)

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

• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump

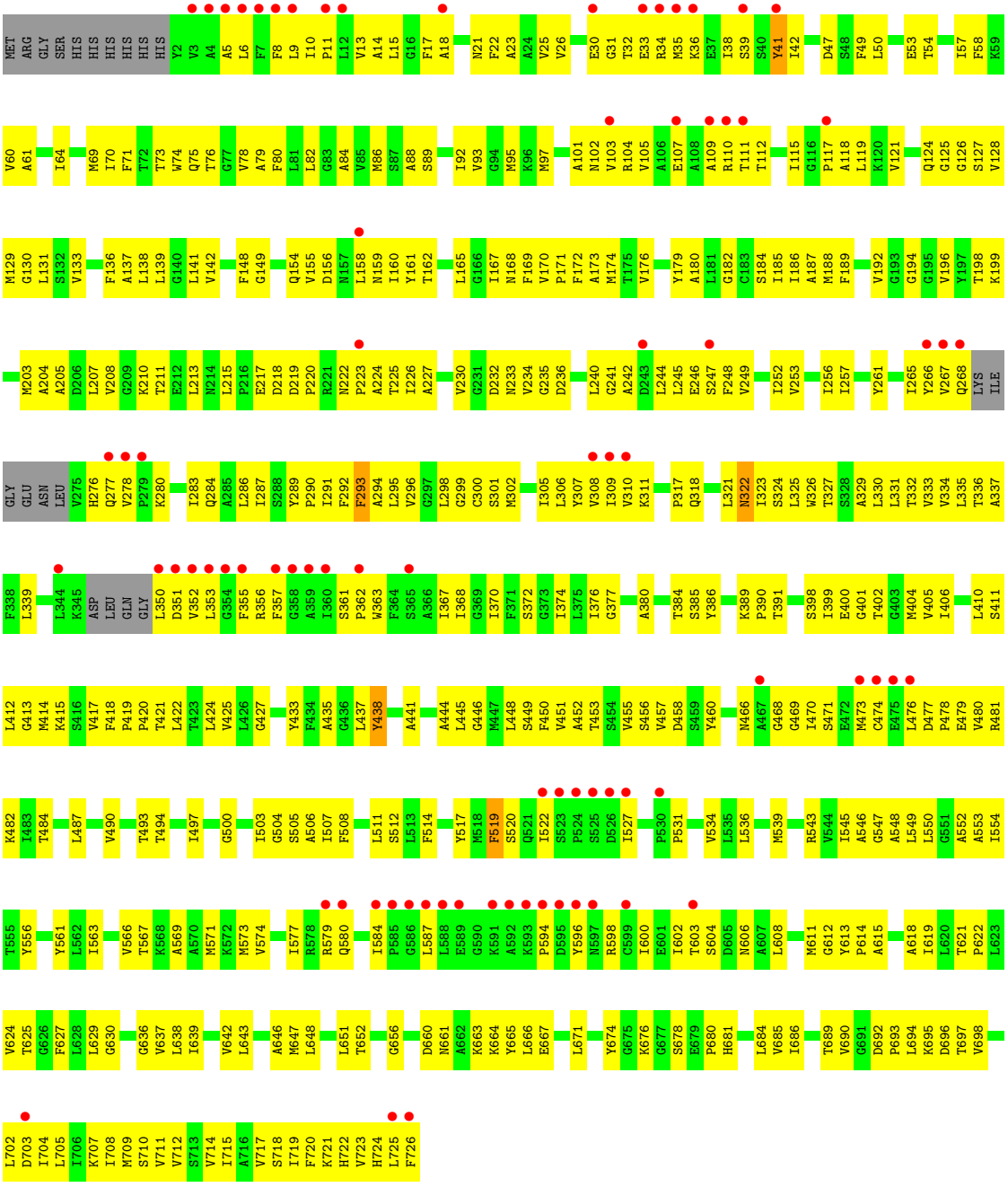
Chain A:





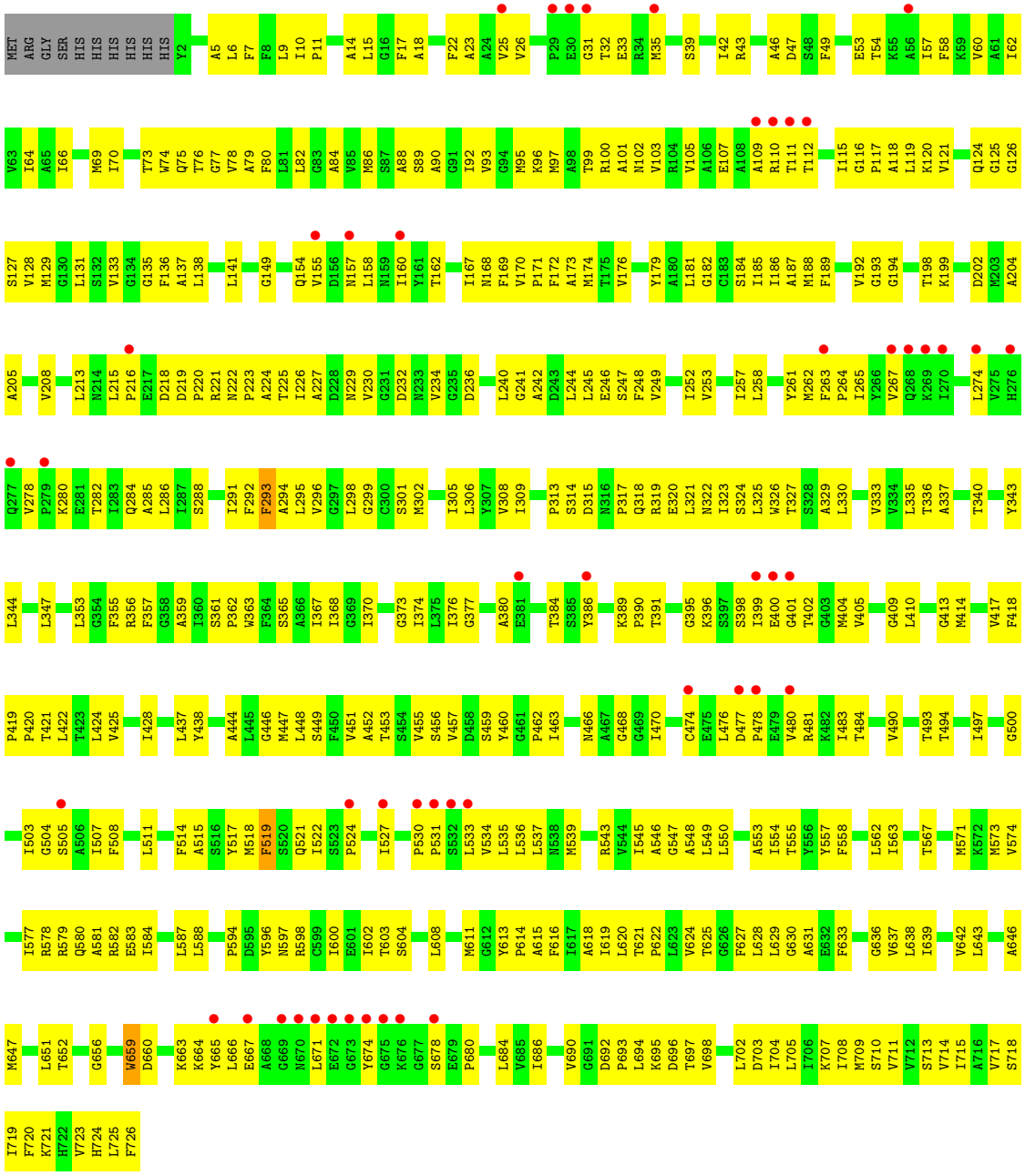
• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump

Chain B:



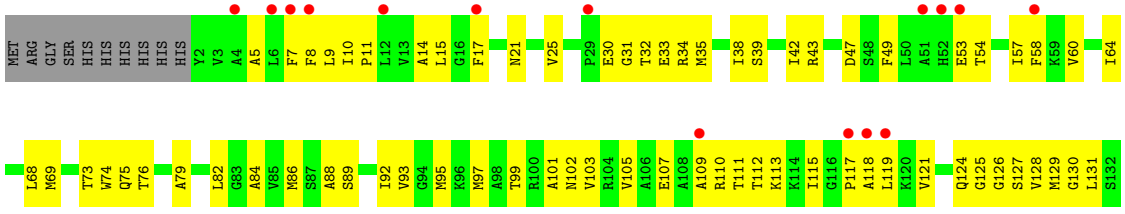
• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump

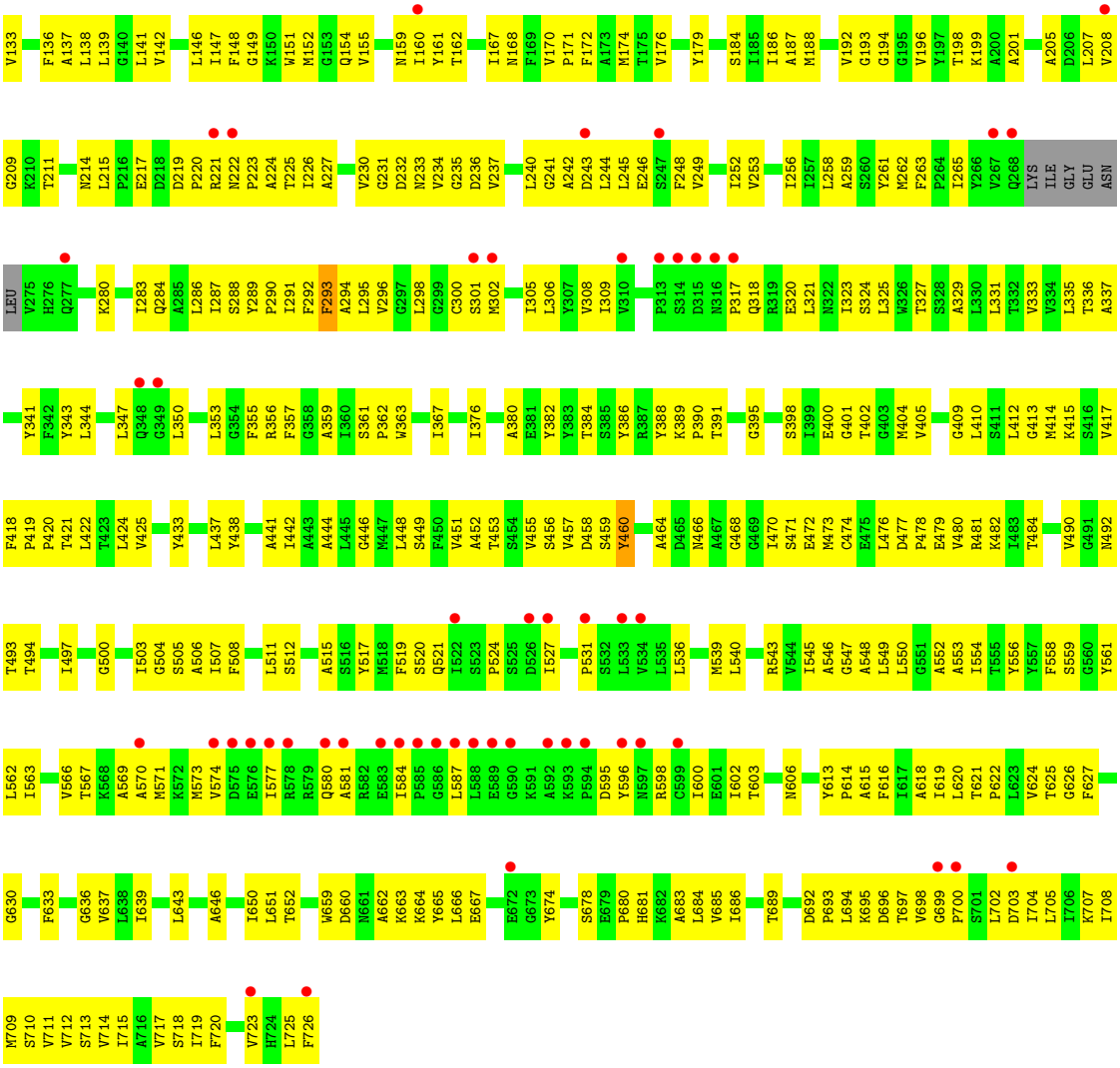
Chain C:



• Molecule 1: K(+)-stimulated pyrophosphate-energized sodium pump

Chain D:




V133 F136 A137 L138 L139 G140 L141 V142 L146 I147 F148 G149 K150 W151 M152 G153 Q154 V155 N159 I160 Y161 T162 I167 N168 F169 V170 P171 F172 A173 M174 T175 V176 Y179 S184 I185 I186 A187 M188 V192 G193 G194 G195 V196 Y197 T198 K199 A200 A201 A205 D206 L207 V208
G209 K210 T211 N214 L215 P216 E217 D218 D219 P220 R221 N222 P223 A224 T225 I226 A227 V230 G231 D232 N233 V234 G235 D236 V237 L240 G241 A242 D243 L244 L245 E246 S247 F248 V249 I252 V253 I256 I257 L258 A259 S260 Y261 M262 F263 P264 I265 Y266 V267 Q268 LYS ILE GLY GLU ASN
LEU V275 H276 Q277 K280 I283 Q284 A285 L286 I287 S288 Y289 P290 I291 F292 F293 A294 L295 V296 G297 L298 G299 C300 S301 M302 I305 L306 Y307 V308 I309 V310 P313 S314 D315 N316 P317 Q318 R319 E320 L321 N322 I323 S324 L325 W326 T327 S328 A329 L330 L331 T332 V333 V334 L335 T336 A337
Y341 F342 Y343 L344 L347 Q348 G349 L350 L353 G354 F355 R356 F357 G358 A359 I360 S361 P362 W363 I367 I376 A380 E381 Y382 Y383 T384 S385 Y386 R387 Y388 K389 P390 T391 G395 S398 I399 E400 G401 T402 G403 M404 V405 G409 L410 S411 L412 G413 M414 K415 S416 V417
F418 P419 P420 T421 L422 T423 L424 V425 Y433 L437 Y438 A441 I442 A443 A444 L445 G446 M447 L448 S449 F450 V451 A452 T453 S454 V455 S456 V457 D458 S459 Y460 A464 D465 N466 A467 G468 G469 I470 S471 E472 M473 C474 E475 L476 D477 P478 E479 V480 R481 K482 I483 T484 V490 G491 N492
T493 T494 I497 G500 I503 G504 S505 A506 I507 F508 L511 S512 A515 S516 Y517 M518 F519 S520 Q521 I522 S523 P524 S525 D526 T527 P531 S532 L533 V534 L535 L536 M539 L540 R543 Y544 I545 A546 G547 A548 L549 L550 G551 A552 A553 I554 T555 Y556 Y557 F558 S559 G560 Y561
L562 I563 V566 T567 K568 A569 A570 M571 K572 M573 V574 D575 E576 I577 R578 R579 Q580 A581 R582 E583 I584 P585 G586 L587 L588 E589 G590 K591 A592 K593 P594 D595 Y596 N597 R598 C599 I600 E601 I602 T603 N606 Y613 P614 A615 F616 I617 A618 I619 L620 T621 P622 L623 V624 T625 G626 F627
G630 F633 G636 V637 L638 I639 L643 A646 I650 L651 T652 W659 D660 N661 A662 K663 K664 Y665 L666 E667 E672 G673 Y674 S678 E679 P680 H681 K682 A683 L684 V685 I686 T689 D692 P693 L694 K695 D696 T697 V698 G699 P700 S701 L702 D703 I704 L705 I706 K707 I708
M709 S710 V711 V712 S713 V714 I715 A716 V717 S718 I719 F720 V723 H724 L725 F726

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.10Å 141.59Å 251.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 3.41 47.48 – 3.41	Depositor EDS
% Data completeness (in resolution range)	74.9 (47.48-3.41) 70.2 (47.48-3.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.228 , 0.284 0.228 , 0.284	Depositor DCC
R_{free} test set	2000 reflections (5.50%)	wwPDB-VP
Wilson B-factor (Å^2)	87.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	21095	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: D1D, 2PN, K, MG, GQB, NA

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	0.25	0/5373	0.39	0/7340
1	B	0.25	0/5289	0.39	0/7223
1	C	0.25	0/5379	0.39	0/7341
1	D	0.25	0/5302	0.39	0/7246
All	All	0.25	0/21343	0.39	0/29150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5260	0	5236	427	0
1	B	5179	0	5167	447	0
1	C	5267	0	5267	466	0
1	D	5189	0	5149	422	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	9	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	1	0	0
3	C	9	0	0	0	0
3	D	9	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	46	30	0	2	0
6	C	23	15	0	0	0
7	C	8	8	8	1	0
8	A	1	0	0	0	0
8	C	3	0	0	1	0
8	D	4	0	0	0	0
All	All	21042	53	20830	1678	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 40.

All (1678) 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:308:VAL:HG21	1:D:324:SER:HB2	1.22	1.16
1:B:32:THR:HG22	1:B:35:MET:HE2	1.28	1.12
1:C:308:VAL:HG21	1:C:324:SER:HB2	1.24	1.09
1:A:14:ALA:HB2	1:A:298:LEU:HD21	1.37	1.06
1:B:308:VAL:HG21	1:B:324:SER:HB2	1.36	1.05
1:C:185:ILE:HG12	1:C:708:ILE:HD11	1.29	1.05
1:B:622:PRO:HG3	1:B:709:MET:HG3	1.38	1.05
1:C:76:THR:HG21	1:C:174:MET:HG3	1.40	1.04
1:C:39:SER:HB3	1:C:103:VAL:HG21	1.38	1.03
1:A:244:LEU:HD23	1:A:455:VAL:HG22	1.39	1.02
1:D:14:ALA:HB2	1:D:298:LEU:HD21	1.40	1.02
1:D:184:SER:HA	1:D:246:GLU:HG3	1.37	1.02
1:A:308:VAL:HG21	1:A:324:SER:HB2	1.42	1.00
1:C:43:ARG:HG2	1:C:99:THR:HB	1.43	1.00
1:C:14:ALA:HB2	1:C:298:LEU:HD21	1.42	0.99
1:B:39:SER:HB3	1:B:103:VAL:HG21	1.44	0.98
1:B:244:LEU:HD23	1:B:455:VAL:HG22	1.44	0.98
1:C:517:TYR:HB2	1:C:714:VAL:HG22	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG22	1:A:121:VAL:HG13	1.46	0.97
1:D:25:VAL:HG11	1:D:97:MET:HE1	1.46	0.96
1:C:244:LEU:HD23	1:C:455:VAL:HG22	1.47	0.96
1:C:622:PRO:HG3	1:C:709:MET:HG3	1.44	0.96
1:D:43:ARG:HG2	1:D:99:THR:HB	1.47	0.96
1:D:468:GLY:CA	1:D:484:THR:HG21	1.95	0.96
1:B:167:ILE:HD11	1:B:719:ILE:HD11	1.45	0.95
1:C:425:VAL:HG13	1:D:546:ALA:HB1	1.49	0.95
1:B:109:ALA:HB2	1:B:118:ALA:HB2	1.48	0.95
1:B:184:SER:HA	1:B:246:GLU:HG3	1.45	0.95
1:D:39:SER:HB3	1:D:103:VAL:HG21	1.45	0.95
1:C:25:VAL:HG11	1:C:97:MET:HE1	1.49	0.95
1:A:39:SER:HB3	1:A:103:VAL:HG21	1.47	0.94
1:B:517:TYR:HB2	1:B:714:VAL:HG22	1.50	0.93
1:A:425:VAL:HG13	1:B:546:ALA:HB1	1.48	0.92
1:B:103:VAL:HG23	1:B:470:ILE:HD13	1.52	0.92
1:C:536:LEU:HD11	1:D:536:LEU:HD11	1.47	0.92
1:D:468:GLY:HA3	1:D:484:THR:HG21	1.51	0.92
1:C:399:ILE:HD11	1:C:671:LEU:HD21	1.50	0.91
1:A:167:ILE:HD11	1:A:719:ILE:HD11	1.51	0.91
1:D:244:LEU:HD23	1:D:455:VAL:HG22	1.50	0.90
1:B:10:ILE:HD12	1:B:295:LEU:HB3	1.52	0.90
1:B:424:LEU:HD23	1:B:507:ILE:HD12	1.51	0.90
1:C:103:VAL:HG23	1:C:470:ILE:HD13	1.54	0.90
1:A:639:ILE:HD13	1:B:539:MET:HG2	1.51	0.90
1:B:110:ARG:HA	1:B:480:VAL:HG22	1.50	0.90
1:A:184:SER:HA	1:A:246:GLU:HG3	1.54	0.89
1:D:31:GLY:HA2	1:D:107:GLU:HG3	1.55	0.89
1:B:105:VAL:HG22	1:B:121:VAL:HG13	1.54	0.89
1:A:622:PRO:HG3	1:A:709:MET:HG3	1.55	0.88
1:A:553:ALA:HB2	1:B:421:THR:HG21	1.56	0.87
1:B:14:ALA:HB2	1:B:298:LEU:HD21	1.54	0.87
1:B:317:PRO:HG2	1:B:490:VAL:HG21	1.55	0.87
1:A:399:ILE:HD11	1:A:671:LEU:HD21	1.57	0.87
1:C:546:ALA:HB1	1:D:425:VAL:HG13	1.55	0.87
1:C:138:LEU:HD13	1:C:295:LEU:HD23	1.57	0.87
1:D:437:LEU:HD13	1:D:515:ALA:HB2	1.55	0.86
1:A:317:PRO:HG2	1:A:490:VAL:HG21	1.57	0.86
1:D:138:LEU:HD13	1:D:295:LEU:HD23	1.56	0.86
1:C:530:PRO:HG2	1:C:533:LEU:HD13	1.57	0.86
1:B:444:ALA:HB2	1:B:508:PHE:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:THR:HG22	1:B:168:ASN:HD22	1.41	0.85
1:A:437:LEU:HD13	1:A:515:ALA:HB2	1.57	0.85
1:C:444:ALA:HB2	1:C:508:PHE:HB3	1.58	0.85
1:C:539:MET:HG2	1:D:539:MET:HG2	1.59	0.85
1:D:105:VAL:HG22	1:D:121:VAL:HG13	1.59	0.84
1:D:160:ILE:HD11	1:D:168:ASN:HB3	1.57	0.84
1:C:79:ALA:HB1	1:C:179:TYR:HB2	1.59	0.84
1:A:539:MET:HG2	1:B:639:ILE:HD13	1.57	0.84
1:B:587:LEU:HD21	1:B:594:PRO:HG3	1.59	0.84
1:A:192:VAL:HG11	1:A:614:PRO:HG3	1.58	0.84
1:D:336:THR:HG22	1:D:363:TRP:HD1	1.41	0.84
1:B:31:GLY:HA2	1:B:107:GLU:HG3	1.60	0.84
1:A:97:MET:HE2	1:A:125:GLY:HA2	1.59	0.83
1:C:105:VAL:HG22	1:C:121:VAL:HG13	1.60	0.83
1:A:306:LEU:HD12	1:A:309:ILE:HD11	1.59	0.83
1:A:138:LEU:HD13	1:A:295:LEU:HD23	1.60	0.83
1:D:517:TYR:HB2	1:D:714:VAL:HG22	1.59	0.83
1:A:639:ILE:CD1	1:B:539:MET:HG2	2.09	0.83
1:D:103:VAL:HG23	1:D:470:ILE:HD13	1.60	0.83
1:B:286:LEU:HB3	1:B:438:TYR:HE2	1.44	0.82
1:B:584:ILE:HG23	1:B:587:LEU:HB2	1.62	0.82
1:C:344:LEU:HD22	1:C:347:LEU:HD11	1.61	0.82
1:B:137:ALA:HB2	1:B:245:LEU:HG	1.60	0.82
1:D:222:ASN:HB3	1:D:225:THR:HG23	1.61	0.82
1:B:399:ILE:HD11	1:B:671:LEU:HD21	1.62	0.82
1:B:308:VAL:HG21	1:B:324:SER:CB	2.10	0.81
1:A:424:LEU:HD23	1:A:507:ILE:HD12	1.59	0.81
1:D:666:LEU:HD11	1:D:680:PRO:HB2	1.63	0.81
1:B:188:MET:HE3	1:B:614:PRO:HB2	1.62	0.81
1:D:39:SER:HB3	1:D:103:VAL:CG2	2.12	0.80
1:D:539:MET:HE2	1:D:639:ILE:HD13	1.62	0.80
1:B:222:ASN:HB3	1:B:225:THR:HG23	1.63	0.80
1:C:199:LYS:HD2	1:C:696:ASP:HB2	1.64	0.80
1:D:492:ASN:ND2	1:D:660:ASP:OD2	2.15	0.80
1:B:580:GLN:O	1:B:584:ILE:HG22	1.80	0.79
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.63	0.79
1:D:308:VAL:HG21	1:D:324:SER:CB	2.07	0.79
1:A:188:MET:HE3	1:A:614:PRO:HB2	1.63	0.79
1:B:32:THR:HG22	1:B:35:MET:CE	2.11	0.79
1:C:39:SER:HB3	1:C:103:VAL:CG2	2.12	0.79
1:B:718:SER:HA	1:B:721:LYS:HD3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:MET:CE	1:C:476:LEU:HD21	2.12	0.79
1:D:110:ARG:HA	1:D:480:VAL:HG22	1.63	0.78
1:A:418:PHE:HB3	1:A:419:PRO:HD3	1.64	0.78
1:C:184:SER:HA	1:C:246:GLU:HG3	1.64	0.78
1:A:325:LEU:HD23	1:A:453:THR:HG22	1.65	0.78
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.66	0.78
1:C:258:LEU:O	1:C:262:MET:HG3	1.84	0.78
1:C:537:LEU:HD23	1:C:639:ILE:HD11	1.64	0.78
1:C:553:ALA:HB2	1:D:421:THR:HG21	1.64	0.78
1:C:76:THR:CG2	1:C:174:MET:HG3	2.14	0.78
1:C:444:ALA:HB2	1:C:508:PHE:CB	2.15	0.77
1:A:222:ASN:HB3	1:A:225:THR:HG23	1.65	0.77
1:B:39:SER:HB3	1:B:103:VAL:CG2	2.14	0.77
1:B:192:VAL:HG11	1:B:614:PRO:HG3	1.64	0.77
1:D:224:ALA:HB2	1:D:577:ILE:HD11	1.66	0.77
1:C:402:THR:HB	1:D:686:ILE:HD13	1.65	0.77
1:C:69:MET:HG2	1:C:74:TRP:HA	1.65	0.76
1:A:424:LEU:HD21	1:A:504:GLY:HA2	1.67	0.76
1:D:472:GLU:HG2	1:D:481:ARG:HD3	1.66	0.76
1:D:347:LEU:HB2	1:D:350:LEU:HD11	1.65	0.76
1:D:444:ALA:HB2	1:D:508:PHE:HB3	1.68	0.76
1:D:320:GLU:O	1:D:323:ILE:HG22	1.86	0.76
1:A:226:ILE:HD12	1:A:596:TYR:CD2	2.21	0.76
1:A:517:TYR:HB2	1:A:714:VAL:HG22	1.69	0.75
1:B:107:GLU:HG2	1:B:110:ARG:HH21	1.51	0.75
1:C:376:ILE:HD11	1:C:424:LEU:CD1	2.16	0.75
1:A:336:THR:HG22	1:A:363:TRP:HD1	1.51	0.75
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.69	0.75
1:C:74:TRP:O	1:C:78:VAL:HG23	1.86	0.75
1:C:448:LEU:HD13	1:C:505:SER:HB2	1.68	0.75
1:A:421:THR:HG21	1:B:553:ALA:HB2	1.68	0.75
1:D:398:SER:HA	1:D:405:VAL:HG22	1.68	0.74
1:A:39:SER:HB3	1:A:103:VAL:CG2	2.17	0.74
1:B:286:LEU:HB3	1:B:438:TYR:CE2	2.21	0.74
1:A:199:LYS:HD2	1:A:696:ASP:HB2	1.68	0.74
1:D:57:ILE:HD13	1:D:186:ILE:HD12	1.70	0.74
1:D:107:GLU:HG2	1:D:110:ARG:HH21	1.52	0.74
1:D:168:ASN:ND2	1:D:718:SER:OG	2.15	0.74
1:D:418:PHE:HB3	1:D:419:PRO:HD3	1.68	0.74
1:A:103:VAL:HG23	1:A:470:ILE:HD13	1.70	0.74
1:B:444:ALA:HB2	1:B:508:PHE:CB	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:MET:HG2	1:B:639:ILE:CD1	2.17	0.74
1:D:79:ALA:HB1	1:D:179:TYR:HB2	1.69	0.74
1:D:137:ALA:HB2	1:D:245:LEU:HG	1.69	0.74
1:A:244:LEU:CD2	1:A:455:VAL:HG22	2.16	0.73
1:D:244:LEU:CD2	1:D:455:VAL:HG22	2.17	0.73
1:D:35:MET:HE2	1:D:476:LEU:HD21	1.69	0.73
1:B:507:ILE:HD11	1:B:646:ALA:HB1	1.70	0.73
1:B:622:PRO:CG	1:B:709:MET:HG3	2.17	0.73
1:C:353:LEU:HD12	1:C:353:LEU:O	1.89	0.73
1:D:353:LEU:HD12	1:D:353:LEU:O	1.88	0.73
1:C:25:VAL:CG1	1:C:97:MET:HE1	2.17	0.73
1:A:10:ILE:HD12	1:A:295:LEU:HB3	1.69	0.73
1:A:74:TRP:O	1:A:78:VAL:HG23	1.88	0.73
1:A:288:SER:HB2	1:A:343:TYR:OH	1.89	0.73
1:C:31:GLY:HA3	1:C:35:MET:SD	2.29	0.73
1:D:286:LEU:HD22	1:D:438:TYR:HE2	1.52	0.73
1:B:126:GLY:O	1:B:456:SER:HA	1.89	0.73
1:A:471:SER:HA	1:A:476:LEU:HD13	1.69	0.72
1:B:138:LEU:HD13	1:B:295:LEU:HD23	1.71	0.72
1:C:424:LEU:HD23	1:C:507:ILE:HD12	1.70	0.72
1:A:353:LEU:HD12	1:A:353:LEU:O	1.89	0.72
1:C:244:LEU:CD2	1:C:455:VAL:HG22	2.19	0.72
1:D:693:PRO:O	1:D:697:THR:OG1	2.06	0.72
1:D:622:PRO:HG3	1:D:709:MET:HG3	1.69	0.72
1:A:594:PRO:HG2	1:A:596:TYR:CE1	2.24	0.72
1:A:137:ALA:HB2	1:A:245:LEU:HG	1.71	0.72
1:A:318:GLN:OE1	1:A:322:ASN:ND2	2.22	0.72
1:B:451:VAL:O	1:B:455:VAL:HG23	1.90	0.72
1:B:336:THR:HG22	1:B:363:TRP:HD1	1.55	0.72
1:A:82:LEU:O	1:A:86:MET:HG2	1.90	0.72
1:C:299:GLY:HA2	1:C:302:MET:HE2	1.72	0.72
1:A:76:THR:OG1	1:A:174:MET:HG3	1.90	0.71
1:A:138:LEU:HD21	1:A:294:ALA:HB1	1.72	0.71
1:B:244:LEU:CD2	1:B:455:VAL:HG22	2.19	0.71
1:A:660:ASP:O	1:A:664:LYS:HG2	1.90	0.71
1:B:105:VAL:HA	1:B:121:VAL:HG11	1.72	0.71
1:B:693:PRO:O	1:B:697:THR:OG1	2.08	0.71
1:C:376:ILE:HD11	1:C:424:LEU:HD11	1.70	0.71
1:A:268:GLN:HG3	1:A:277:GLN:HE21	1.54	0.71
1:A:522:ILE:HD11	1:A:534:VAL:HG11	1.72	0.71
1:A:329:ALA:O	1:A:333:VAL:HG23	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LEU:HD11	1:B:536:LEU:HD11	1.72	0.71
1:A:543:ARG:HH12	1:A:629:LEU:HD22	1.55	0.71
1:A:686:ILE:HD13	1:B:402:THR:HB	1.72	0.71
1:B:424:LEU:CD2	1:B:507:ILE:HD12	2.21	0.71
1:C:363:TRP:CE2	1:C:367:ILE:HD11	2.26	0.71
1:B:69:MET:HG2	1:B:74:TRP:HA	1.71	0.71
1:B:168:ASN:H	1:B:718:SER:CB	2.04	0.71
1:A:49:PHE:CD1	1:A:234:VAL:HG11	2.26	0.71
1:C:511:LEU:HD12	1:D:545:ILE:HD13	1.73	0.71
1:C:539:MET:HG3	1:D:539:MET:HE2	1.71	0.71
1:C:329:ALA:O	1:C:333:VAL:HG23	1.90	0.70
1:A:380:ALA:O	1:A:384:THR:HG22	1.91	0.70
1:C:336:THR:HG22	1:C:363:TRP:HD1	1.55	0.70
1:A:208:VAL:HG22	1:A:574:VAL:HG13	1.73	0.70
1:A:377:GLY:HA2	1:A:497:ILE:HG23	1.73	0.70
1:B:448:LEU:HD13	1:B:505:SER:HB2	1.74	0.70
1:D:194:GLY:HA3	1:D:235:GLY:HA2	1.73	0.70
1:D:437:LEU:HD13	1:D:515:ALA:CB	2.21	0.70
1:B:301:SER:CB	1:B:452:ALA:HB3	2.21	0.70
1:C:35:MET:HE1	1:C:476:LEU:HD21	1.73	0.70
1:B:138:LEU:HD12	1:B:298:LEU:HD13	1.74	0.70
1:A:10:ILE:HG22	1:A:298:LEU:HD22	1.74	0.70
1:C:262:MET:HE1	1:C:353:LEU:HB2	1.73	0.70
1:D:8:PHE:CE2	1:D:146:LEU:HD21	2.26	0.70
1:D:31:GLY:HA3	1:D:35:MET:SD	2.31	0.70
1:D:103:VAL:CG2	1:D:470:ILE:HD13	2.21	0.70
1:D:336:THR:HG22	1:D:363:TRP:CD1	2.27	0.70
1:A:545:ILE:HG21	1:B:511:LEU:HD11	1.73	0.70
1:B:110:ARG:HA	1:B:480:VAL:CG2	2.22	0.70
1:B:608:LEU:HA	1:B:611:MET:HE2	1.73	0.70
1:B:627:PHE:CD1	1:B:720:PHE:HB3	2.27	0.69
1:D:105:VAL:HG22	1:D:121:VAL:CG1	2.22	0.69
1:A:35:MET:CE	1:A:476:LEU:HD21	2.23	0.69
1:D:347:LEU:HB2	1:D:350:LEU:CD1	2.22	0.69
1:A:471:SER:CB	1:A:476:LEU:HD22	2.22	0.69
1:B:103:VAL:CG2	1:B:470:ILE:HD13	2.22	0.69
1:C:355:PHE:CD1	1:C:362:PRO:HD3	2.27	0.69
1:C:584:ILE:HG22	1:C:587:LEU:HB2	1.74	0.69
1:A:208:VAL:CG2	1:A:574:VAL:HG13	2.23	0.69
1:B:112:THR:HG21	1:B:117:PRO:HG2	1.73	0.69
1:A:224:ALA:HB2	1:A:577:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:THR:HG21	1:D:553:ALA:HB2	1.75	0.69
1:B:199:LYS:HD2	1:B:696:ASP:HB2	1.74	0.69
1:D:451:VAL:O	1:D:455:VAL:HG23	1.92	0.69
1:B:189:PHE:HE1	1:B:612:GLY:HA2	1.57	0.69
1:C:414:MET:HG2	1:C:651:LEU:HD11	1.75	0.69
1:D:76:THR:OG1	1:D:174:MET:HG3	1.93	0.69
1:D:82:LEU:O	1:D:86:MET:HG2	1.93	0.69
1:A:400:GLU:HG3	1:B:571:MET:HG2	1.74	0.69
1:A:451:VAL:O	1:A:455:VAL:HG23	1.93	0.69
1:B:353:LEU:HD12	1:B:353:LEU:O	1.92	0.69
1:B:522:ILE:HD11	1:B:534:VAL:HG11	1.73	0.69
1:D:25:VAL:CG1	1:D:97:MET:HE1	2.21	0.69
1:D:35:MET:CE	1:D:476:LEU:HD21	2.23	0.69
1:C:424:LEU:HD21	1:C:504:GLY:HA2	1.75	0.69
1:B:82:LEU:O	1:B:86:MET:HG2	1.93	0.68
1:C:105:VAL:HA	1:C:121:VAL:HG11	1.75	0.68
1:C:222:ASN:HB3	1:C:225:THR:HG23	1.75	0.68
1:D:199:LYS:HD2	1:D:696:ASP:HB2	1.74	0.68
1:A:545:ILE:HD13	1:B:511:LEU:HD12	1.74	0.68
1:C:325:LEU:HD23	1:C:453:THR:HG22	1.75	0.68
1:A:717:VAL:HA	1:A:720:PHE:CZ	2.28	0.68
1:C:138:LEU:HD12	1:C:298:LEU:HD13	1.74	0.68
1:C:167:ILE:HD11	1:C:719:ILE:HD11	1.75	0.68
1:D:133:VAL:HG13	1:D:245:LEU:HB2	1.75	0.68
1:B:49:PHE:CD1	1:B:234:VAL:HG11	2.28	0.68
1:B:199:LYS:HD3	1:B:692:ASP:HB3	1.73	0.68
1:C:14:ALA:CB	1:C:298:LEU:HD21	2.20	0.68
1:C:172:PHE:O	1:C:176:VAL:HG22	1.94	0.68
1:A:5:ALA:O	1:A:9:LEU:HD13	1.94	0.68
1:C:545:ILE:HD13	1:D:511:LEU:HD12	1.75	0.68
1:C:545:ILE:HG21	1:D:511:LEU:HD11	1.76	0.68
1:C:261:TYR:O	1:C:265:ILE:HD13	1.93	0.67
1:C:337:ALA:HB2	1:C:363:TRP:CE2	2.29	0.67
1:C:660:ASP:O	1:C:664:LYS:HG2	1.95	0.67
1:D:243:ASP:CG	1:D:704:ILE:HD11	2.14	0.67
1:D:259:ALA:HA	1:D:262:MET:HE2	1.75	0.67
1:A:109:ALA:HB2	1:A:118:ALA:HB2	1.76	0.67
1:B:10:ILE:HG22	1:B:298:LEU:HD22	1.76	0.67
1:B:138:LEU:HD21	1:B:294:ALA:HB1	1.76	0.67
1:A:299:GLY:HA2	1:A:302:MET:HE2	1.76	0.67
1:A:437:LEU:HD13	1:A:515:ALA:CB	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:MET:HE1	1:C:241:GLY:H	1.59	0.67
1:B:596:TYR:O	1:B:600:ILE:HG12	1.95	0.67
1:D:448:LEU:HD13	1:D:505:SER:HB3	1.77	0.67
1:D:627:PHE:CD1	1:D:720:PHE:HB3	2.29	0.67
1:C:451:VAL:O	1:C:455:VAL:HG23	1.95	0.67
1:C:490:VAL:O	1:C:494:THR:HG23	1.94	0.67
1:A:58:PHE:O	1:A:62:ILE:HD13	1.96	0.66
1:B:26:VAL:HA	1:B:104:ARG:CZ	2.25	0.66
1:B:79:ALA:HB1	1:B:179:TYR:HB2	1.77	0.66
1:C:124:GLN:O	1:C:128:VAL:HG23	1.95	0.66
1:C:598:ARG:O	1:C:602:ILE:HG12	1.95	0.66
1:A:149:GLY:CA	1:A:155:VAL:HG23	2.25	0.66
1:C:414:MET:HG2	1:C:651:LEU:CD1	2.26	0.66
1:A:84:ALA:HA	1:A:186:ILE:HG13	1.77	0.66
1:B:413:GLY:O	1:B:417:VAL:HG23	1.95	0.66
1:C:293:PHE:CE2	1:C:336:THR:HG21	2.31	0.66
1:D:38:ILE:HD12	1:D:473:MET:HE1	1.78	0.66
1:B:199:LYS:HE2	1:B:199:LYS:HA	1.77	0.66
1:C:84:ALA:CB	1:C:186:ILE:HG13	2.26	0.66
1:C:318:GLN:OE1	1:C:322:ASN:ND2	2.23	0.66
1:C:545:ILE:HD13	1:D:511:LEU:CD1	2.25	0.66
1:A:507:ILE:HD11	1:A:646:ALA:CB	2.25	0.66
1:B:162:THR:HG22	1:B:168:ASN:ND2	2.08	0.66
1:B:105:VAL:HG22	1:B:121:VAL:CG1	2.23	0.66
1:D:168:ASN:HD22	1:D:718:SER:HG	1.40	0.66
1:B:711:VAL:O	1:B:715:ILE:HG23	1.95	0.66
1:C:208:VAL:HG22	1:C:574:VAL:HG13	1.78	0.66
1:C:265:ILE:HG21	1:C:519:PHE:CE1	2.31	0.66
1:B:109:ALA:HB2	1:B:118:ALA:CB	2.26	0.66
1:A:598:ARG:O	1:A:602:ILE:HG12	1.96	0.65
1:B:676:LYS:O	1:B:681:HIS:ND1	2.20	0.65
1:C:73:THR:OG1	1:C:76:THR:HG23	1.97	0.65
1:C:116:GLY:CA	1:C:313:PRO:HB2	2.26	0.65
1:C:686:ILE:HD13	1:D:402:THR:HB	1.79	0.65
1:D:5:ALA:O	1:D:9:LEU:HD13	1.95	0.65
1:C:292:PHE:O	1:C:296:VAL:HG23	1.96	0.65
1:D:619:ILE:HG12	1:D:708:ILE:HD11	1.78	0.65
1:C:548:ALA:HA	1:C:636:GLY:O	1.96	0.65
1:C:126:GLY:O	1:C:456:SER:HA	1.96	0.65
1:C:185:ILE:CG1	1:C:708:ILE:HD11	2.16	0.65
1:A:492:ASN:ND2	1:A:660:ASP:OD2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.31	0.65
1:C:318:GLN:O	1:C:322:ASN:ND2	2.27	0.65
1:C:587:LEU:HD21	1:C:594:PRO:HG3	1.78	0.65
1:D:14:ALA:CB	1:D:298:LEU:HD21	2.20	0.65
1:A:573:MET:SD	1:A:603:THR:HG23	2.37	0.65
1:B:156:ASP:O	1:B:280:LYS:HD3	1.97	0.65
1:D:471:SER:HA	1:D:476:LEU:HD13	1.80	0.65
1:A:652:THR:HB	1:A:694:LEU:O	1.97	0.64
1:C:643:LEU:HD12	1:D:643:LEU:HD12	1.79	0.64
1:A:293:PHE:CE2	1:A:336:THR:HG21	2.32	0.64
1:D:259:ALA:HA	1:D:262:MET:CE	2.27	0.64
1:C:247:SER:HA	1:C:707:LYS:HE3	1.79	0.64
1:A:530:PRO:HG2	1:A:533:LEU:HD13	1.79	0.64
1:B:329:ALA:O	1:B:333:VAL:HG23	1.97	0.64
1:C:102:ASN:OD1	1:C:103:VAL:N	2.31	0.64
1:C:507:ILE:HG21	1:D:549:LEU:HD11	1.78	0.64
1:D:199:LYS:HA	1:D:199:LYS:HE2	1.80	0.64
1:C:627:PHE:CD1	1:C:720:PHE:HB3	2.32	0.64
1:D:248:PHE:CZ	1:D:294:ALA:HB1	2.33	0.64
1:A:103:VAL:CG2	1:A:470:ILE:HD13	2.27	0.64
1:A:336:THR:HG22	1:A:363:TRP:CD1	2.32	0.64
1:A:666:LEU:HD23	1:A:666:LEU:O	1.98	0.64
1:B:507:ILE:HD11	1:B:646:ALA:CB	2.27	0.64
1:C:507:ILE:HD11	1:C:646:ALA:HB1	1.78	0.64
1:D:188:MET:HB2	1:D:704:ILE:CG2	2.27	0.64
1:B:703:ASP:OD1	1:B:704:ILE:N	2.31	0.64
1:B:172:PHE:O	1:B:176:VAL:HG22	1.97	0.64
1:B:712:VAL:O	1:B:715:ILE:HG13	1.98	0.64
1:C:424:LEU:CD2	1:C:507:ILE:HD12	2.27	0.64
1:C:543:ARG:HH12	1:C:629:LEU:HD22	1.61	0.63
1:D:329:ALA:O	1:D:333:VAL:HG23	1.97	0.63
1:A:35:MET:HE2	1:A:476:LEU:HD21	1.78	0.63
1:A:444:ALA:HB2	1:A:508:PHE:HB3	1.81	0.63
1:C:703:ASP:OD1	1:C:704:ILE:N	2.30	0.63
1:D:413:GLY:O	1:D:417:VAL:HG23	1.99	0.63
1:B:268:GLN:HG3	1:B:277:GLN:HE21	1.63	0.63
1:C:192:VAL:HG11	1:C:614:PRO:HG3	1.79	0.63
1:D:265:ILE:HG22	1:D:531:PRO:HG3	1.80	0.63
1:B:421:THR:O	1:B:425:VAL:HG23	1.98	0.63
1:C:308:VAL:HG21	1:C:324:SER:CB	2.15	0.63
1:D:188:MET:HB2	1:D:704:ILE:HG21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ILE:HD11	1:A:646:ALA:HB1	1.80	0.63
1:B:102:ASN:OD1	1:B:103:VAL:N	2.32	0.63
1:A:105:VAL:HG22	1:A:121:VAL:CG1	2.26	0.63
1:B:208:VAL:HG11	1:B:577:ILE:CG2	2.28	0.63
1:C:84:ALA:HB1	1:C:186:ILE:HG13	1.80	0.63
1:D:138:LEU:HD21	1:D:294:ALA:HB1	1.81	0.63
1:D:258:LEU:O	1:D:262:MET:HG3	1.98	0.63
1:D:355:PHE:CD1	1:D:362:PRO:HD3	2.33	0.63
1:A:14:ALA:CB	1:A:298:LEU:HD21	2.22	0.63
1:C:11:PRO:O	1:C:15:LEU:HG	1.99	0.63
1:C:666:LEU:HD23	1:C:666:LEU:O	1.99	0.63
1:A:177:SER:HB3	1:A:715:ILE:HD11	1.80	0.63
1:C:138:LEU:HD12	1:C:298:LEU:CD1	2.29	0.63
1:C:286:LEU:HB3	1:C:438:TYR:CE2	2.34	0.63
1:C:301:SER:CB	1:C:452:ALA:HB3	2.29	0.63
1:C:112:THR:CB	1:C:117:PRO:HG2	2.29	0.62
1:D:68:LEU:HD13	1:D:76:THR:HG22	1.81	0.62
1:A:172:PHE:O	1:A:176:VAL:HG22	1.99	0.62
1:C:399:ILE:HD13	1:C:680:PRO:HB3	1.81	0.62
1:A:43:ARG:HG3	1:A:99:THR:HB	1.82	0.62
1:A:703:ASP:OD1	1:A:704:ILE:N	2.32	0.62
1:B:666:LEU:O	1:B:666:LEU:HD23	1.99	0.62
1:C:82:LEU:O	1:C:86:MET:HG2	1.99	0.62
1:C:380:ALA:O	1:C:384:THR:HG22	1.99	0.62
1:B:380:ALA:O	1:B:384:THR:HG22	2.00	0.62
1:D:172:PHE:O	1:D:176:VAL:HG22	2.00	0.62
1:D:414:MET:HG2	1:D:651:LEU:CD1	2.29	0.62
1:A:222:ASN:HB3	1:A:225:THR:CG2	2.30	0.62
1:D:301:SER:CB	1:D:452:ALA:HB3	2.29	0.62
1:A:424:LEU:CD2	1:A:507:ILE:HD12	2.30	0.62
1:A:105:VAL:HA	1:A:121:VAL:HG11	1.82	0.62
1:C:622:PRO:CG	1:C:709:MET:HG3	2.27	0.62
1:D:507:ILE:HD11	1:D:646:ALA:HB1	1.81	0.62
1:A:321:LEU:HD13	1:A:457:VAL:HG13	1.80	0.62
1:A:25:VAL:HG21	1:A:97:MET:HE1	1.82	0.61
1:A:448:LEU:HD13	1:A:505:SER:HB2	1.82	0.61
1:D:380:ALA:O	1:D:384:THR:HG22	1.99	0.61
1:B:73:THR:HB	1:B:75:GLN:OE1	2.00	0.61
1:C:176:VAL:HB	1:C:253:VAL:HG13	1.82	0.61
1:C:514:PHE:CE1	1:C:638:LEU:HB3	2.35	0.61
1:B:168:ASN:H	1:B:718:SER:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLY:HA2	1:B:302:MET:HE2	1.81	0.61
1:C:363:TRP:CZ2	1:C:367:ILE:HD11	2.35	0.61
1:A:11:PRO:HD3	1:A:295:LEU:HD22	1.82	0.61
1:A:247:SER:HA	1:A:707:LYS:HE3	1.80	0.61
1:D:110:ARG:HA	1:D:480:VAL:CG2	2.29	0.61
1:B:138:LEU:HD12	1:B:298:LEU:CD1	2.31	0.61
1:A:545:ILE:HD13	1:B:511:LEU:CD1	2.30	0.61
1:B:105:VAL:HG22	1:B:121:VAL:HG22	1.82	0.61
1:B:300:CYS:SG	1:B:335:LEU:HD22	2.40	0.61
1:C:344:LEU:HD22	1:C:347:LEU:CD1	2.29	0.61
1:D:256:ILE:HG23	1:D:287:ILE:HG23	1.82	0.61
1:D:292:PHE:O	1:D:296:VAL:HG23	2.00	0.61
1:A:444:ALA:HB2	1:A:508:PHE:CB	2.31	0.61
1:A:573:MET:CE	1:A:599:CYS:HB3	2.31	0.61
1:C:267:VAL:HG11	1:C:274:LEU:HB3	1.81	0.61
1:B:84:ALA:CB	1:B:186:ILE:HG13	2.31	0.61
1:B:112:THR:CB	1:B:117:PRO:HG2	2.31	0.61
1:B:309:ILE:HD12	1:B:310:VAL:HG23	1.83	0.61
1:A:507:ILE:HG21	1:B:549:LEU:HD11	1.83	0.61
1:B:124:GLN:O	1:B:128:VAL:HG23	2.01	0.61
1:B:176:VAL:HB	1:B:253:VAL:HG13	1.83	0.61
1:D:301:SER:HB3	1:D:452:ALA:HB3	1.83	0.61
1:A:42:ILE:HD12	1:A:43:ARG:N	2.16	0.61
1:A:710:SER:O	1:A:714:VAL:HG23	2.01	0.61
1:A:199:LYS:HA	1:A:199:LYS:HE2	1.83	0.60
1:B:336:THR:HG22	1:B:363:TRP:CD1	2.36	0.60
1:C:232:ASP:O	1:C:236:ASP:HB2	2.01	0.60
1:C:530:PRO:CG	1:C:533:LEU:HD13	2.30	0.60
1:A:191:ARG:NH1	1:A:235:GLY:O	2.34	0.60
1:A:376:ILE:HD11	1:A:424:LEU:HD11	1.83	0.60
1:B:256:ILE:HG23	1:B:287:ILE:HG23	1.83	0.60
1:B:584:ILE:CG2	1:B:587:LEU:HB2	2.29	0.60
1:C:314:SER:HB2	1:C:320:GLU:OE2	2.02	0.60
1:D:127:SER:OG	1:D:305:ILE:HG21	2.01	0.60
1:D:548:ALA:HA	1:D:636:GLY:O	2.01	0.60
1:A:344:LEU:HD22	1:A:347:LEU:HD11	1.84	0.60
1:A:480:VAL:O	1:A:484:THR:HG23	2.00	0.60
1:B:169:PHE:HB2	1:B:174:MET:HE3	1.82	0.60
1:B:292:PHE:O	1:B:296:VAL:HG23	2.01	0.60
1:B:321:LEU:HD13	1:B:457:VAL:HG13	1.82	0.60
1:C:400:GLU:HB2	1:C:404:MET:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:LEU:HD22	1:C:726:PHE:CZ	2.36	0.60
1:A:213:LEU:HB3	1:A:215:LEU:HD13	1.83	0.60
1:C:119:LEU:HD21	1:C:320:GLU:HG3	1.83	0.60
1:D:138:LEU:HD12	1:D:298:LEU:HD13	1.84	0.60
1:B:474:CYS:HB2	1:B:476:LEU:CD1	2.32	0.60
1:B:598:ARG:O	1:B:602:ILE:HG12	2.01	0.60
1:C:73:THR:O	1:C:76:THR:OG1	2.13	0.60
1:D:363:TRP:CE2	1:D:367:ILE:HD11	2.37	0.60
1:D:703:ASP:OD1	1:D:704:ILE:N	2.34	0.60
1:A:306:LEU:CD1	1:A:309:ILE:HD11	2.31	0.60
1:A:347:LEU:HB2	1:A:350:LEU:CD1	2.32	0.60
1:D:117:PRO:O	1:D:121:VAL:HG12	2.02	0.60
1:B:240:LEU:HD12	1:B:244:LEU:HD13	1.83	0.60
1:C:69:MET:HG3	1:C:77:GLY:HA3	1.84	0.60
1:C:563:ILE:O	1:C:567:THR:HG23	2.01	0.60
1:D:141:LEU:HD21	1:D:252:ILE:HG21	1.84	0.60
1:D:261:TYR:CE1	1:D:520:SER:HA	2.37	0.60
1:A:376:ILE:HD11	1:A:424:LEU:CD1	2.32	0.59
1:A:556:TYR:OH	1:B:556:TYR:OH	2.16	0.59
1:B:331:LEU:O	1:B:335:LEU:HD13	2.02	0.59
1:B:386:TYR:CD2	1:B:665:TYR:HB2	2.37	0.59
1:D:84:ALA:HA	1:D:186:ILE:HG13	1.82	0.59
1:D:444:ALA:HB2	1:D:508:PHE:CB	2.31	0.59
1:D:490:VAL:O	1:D:494:THR:HG23	2.02	0.59
1:D:596:TYR:O	1:D:600:ILE:HG12	2.02	0.59
1:B:223:PRO:HG2	1:B:577:ILE:HG12	1.84	0.59
1:A:446:GLY:HA2	1:A:449:SER:HB3	1.83	0.59
1:C:674:TYR:CD2	1:C:680:PRO:HG2	2.37	0.59
1:D:31:GLY:HA2	1:D:107:GLU:CG	2.31	0.59
1:D:69:MET:HG2	1:D:74:TRP:HA	1.84	0.59
1:D:217:GLU:OE2	1:D:663:LYS:NZ	2.35	0.59
1:D:563:ILE:O	1:D:567:THR:HG23	2.02	0.59
1:A:355:PHE:CD1	1:A:362:PRO:HD3	2.37	0.59
1:C:18:ALA:HB2	1:C:131:LEU:HB2	1.84	0.59
1:C:437:LEU:HD13	1:C:515:ALA:HB2	1.84	0.59
1:A:57:ILE:CD1	1:A:189:PHE:HB3	2.32	0.59
1:A:79:ALA:HB1	1:A:179:TYR:HB2	1.85	0.59
1:B:718:SER:O	1:B:721:LYS:HE3	2.03	0.59
1:C:10:ILE:HD12	1:C:295:LEU:HB3	1.84	0.59
1:D:187:ALA:HA	1:D:242:ALA:HB1	1.85	0.59
1:A:37:GLU:O	1:A:41:TYR:HD1	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TYR:HH	1:A:288:SER:HG	1.50	0.59
1:A:292:PHE:O	1:A:296:VAL:HG23	2.03	0.59
1:A:398:SER:HA	1:A:405:VAL:HG22	1.83	0.59
1:C:446:GLY:HA2	1:C:449:SER:HB3	1.83	0.59
1:D:73:THR:HB	1:D:75:GLN:OE1	2.03	0.59
1:A:428:ILE:HG13	1:A:508:PHE:HE1	1.67	0.59
1:C:103:VAL:CG2	1:C:470:ILE:HD13	2.30	0.59
1:D:507:ILE:HD11	1:D:646:ALA:CB	2.32	0.59
1:C:507:ILE:HD11	1:C:646:ALA:CB	2.33	0.59
1:D:112:THR:CB	1:D:117:PRO:HG2	2.33	0.59
1:D:199:LYS:HD3	1:D:692:ASP:HB3	1.84	0.59
1:A:725:LEU:HD23	1:A:725:LEU:O	2.02	0.59
1:B:301:SER:HB2	1:B:452:ALA:HB3	1.85	0.59
1:C:571:MET:HG3	1:D:404:MET:CE	2.33	0.59
1:A:400:GLU:HB2	1:A:404:MET:HG3	1.85	0.58
1:B:160:ILE:O	1:B:160:ILE:HG23	2.02	0.58
1:D:148:PHE:O	1:D:154:GLN:HB2	2.03	0.58
1:A:124:GLN:O	1:A:128:VAL:HG23	2.03	0.58
1:A:268:GLN:CG	1:A:277:GLN:HE21	2.15	0.58
1:B:522:ILE:HD11	1:B:534:VAL:HG21	1.85	0.58
1:C:10:ILE:HG22	1:C:298:LEU:HD22	1.85	0.58
1:C:208:VAL:HG21	1:C:574:VAL:HA	1.85	0.58
1:D:474:CYS:HB2	1:D:476:LEU:CD1	2.33	0.58
1:A:127:SER:OG	1:A:305:ILE:HG21	2.03	0.58
1:A:293:PHE:CZ	1:A:336:THR:HG21	2.38	0.58
1:B:490:VAL:O	1:B:494:THR:HG23	2.03	0.58
1:C:25:VAL:CB	1:C:97:MET:HE1	2.33	0.58
1:C:120:LYS:HG3	1:C:313:PRO:HB3	1.85	0.58
1:C:511:LEU:HD11	1:D:545:ILE:HG21	1.85	0.58
1:A:548:ALA:HA	1:A:636:GLY:O	2.03	0.58
1:B:261:TYR:CE1	1:B:520:SER:HA	2.38	0.58
1:C:160:ILE:HG23	1:C:160:ILE:O	2.03	0.58
1:D:110:ARG:O	1:D:113:LYS:NZ	2.37	0.58
1:C:199:LYS:HE2	1:C:199:LYS:HA	1.84	0.58
1:C:218:ASP:HA	1:C:225:THR:HG22	1.85	0.58
1:C:717:VAL:HA	1:C:720:PHE:CE1	2.37	0.58
1:A:102:ASN:OD1	1:A:103:VAL:N	2.36	0.58
1:A:401:GLY:HA3	1:B:207:LEU:HD21	1.86	0.58
1:B:103:VAL:HG22	1:B:470:ILE:HG21	1.85	0.58
1:D:666:LEU:O	1:D:666:LEU:HD23	2.03	0.58
1:B:204:ALA:HB3	1:B:573:MET:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:VAL:HG22	1:C:121:VAL:CG1	2.33	0.58
1:D:619:ILE:CG1	1:D:708:ILE:HD11	2.34	0.58
1:A:89:SER:O	1:A:93:VAL:HG23	2.04	0.58
1:B:84:ALA:HA	1:B:186:ILE:HG13	1.86	0.58
1:C:511:LEU:CD1	1:D:545:ILE:HD13	2.33	0.58
1:C:517:TYR:OH	1:C:631:ALA:O	2.22	0.58
1:D:188:MET:HE3	1:D:614:PRO:HB2	1.86	0.58
1:B:268:GLN:CG	1:B:277:GLN:HE21	2.16	0.58
1:B:326:TRP:O	1:B:330:LEU:HD13	2.04	0.58
1:B:356:ARG:HD2	1:B:433:TYR:O	2.04	0.58
1:C:73:THR:HB	1:C:75:GLN:OE1	2.04	0.58
1:D:695:LYS:NZ	1:D:696:ASP:OD2	2.36	0.58
1:A:413:GLY:O	1:A:417:VAL:HG23	2.03	0.57
1:B:26:VAL:HA	1:B:104:ARG:NH1	2.18	0.57
1:B:75:GLN:HA	1:B:78:VAL:CG2	2.33	0.57
1:B:548:ALA:HA	1:B:636:GLY:O	2.04	0.57
1:B:622:PRO:HG3	1:B:709:MET:CG	2.23	0.57
1:D:11:PRO:O	1:D:15:LEU:HG	2.03	0.57
1:D:112:THR:OG1	1:D:117:PRO:HG2	2.04	0.57
1:A:31:GLY:HA3	1:A:35:MET:SD	2.44	0.57
1:A:84:ALA:CA	1:A:186:ILE:HG13	2.34	0.57
1:A:514:PHE:CE1	1:A:638:LEU:HB3	2.39	0.57
1:C:49:PHE:CD1	1:C:234:VAL:HG11	2.39	0.57
1:C:418:PHE:HE2	1:D:554:ILE:HG12	1.69	0.57
1:C:652:THR:HB	1:C:694:LEU:O	2.04	0.57
1:B:75:GLN:HA	1:B:78:VAL:HG22	1.86	0.57
1:C:7:PHE:O	1:C:10:ILE:HG13	2.04	0.57
1:C:57:ILE:CD1	1:C:189:PHE:HB3	2.35	0.57
1:C:474:CYS:HB2	1:C:476:LEU:CD1	2.33	0.57
1:D:219:ASP:O	1:D:225:THR:HG21	2.04	0.57
1:A:240:LEU:HD12	1:A:244:LEU:HD13	1.87	0.57
1:A:471:SER:HB2	1:A:476:LEU:HD22	1.85	0.57
1:A:522:ILE:HD11	1:A:534:VAL:HG21	1.87	0.57
1:B:222:ASN:HB3	1:B:225:THR:CG2	2.33	0.57
1:B:337:ALA:HB2	1:B:363:TRP:CE2	2.39	0.57
1:C:413:GLY:O	1:C:417:VAL:HG23	2.03	0.57
1:D:471:SER:CB	1:D:476:LEU:HD22	2.35	0.57
1:D:558:PHE:CE1	1:D:562:LEU:HD11	2.39	0.57
1:B:265:ILE:HG21	1:B:519:PHE:CE1	2.39	0.57
1:C:116:GLY:O	1:C:120:LYS:HG3	2.03	0.57
1:C:199:LYS:HD3	1:C:692:ASP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:MET:HG2	1:D:651:LEU:HD12	1.85	0.57
1:A:573:MET:HE1	1:A:599:CYS:HB3	1.86	0.57
1:C:340:THR:CG2	1:C:362:PRO:HG2	2.34	0.57
1:C:725:LEU:O	1:C:725:LEU:HD23	2.04	0.57
1:D:49:PHE:CD1	1:D:234:VAL:HG11	2.40	0.57
1:D:263:PHE:CZ	1:D:280:LYS:HE2	2.39	0.57
1:D:288:SER:OG	1:D:343:TYR:OH	1.97	0.57
1:A:138:LEU:HD21	1:A:294:ALA:CB	2.34	0.57
1:B:167:ILE:CD1	1:B:719:ILE:HD11	2.28	0.57
1:B:208:VAL:HG22	1:B:574:VAL:HG13	1.86	0.57
1:C:299:GLY:HA2	1:C:302:MET:CE	2.35	0.57
1:C:344:LEU:CD2	1:C:347:LEU:HD11	2.33	0.57
1:D:700:PRO:O	1:D:704:ILE:HD12	2.05	0.57
1:A:148:PHE:O	1:A:154:GLN:HB2	2.05	0.57
1:A:331:LEU:O	1:A:335:LEU:HD13	2.05	0.57
1:A:490:VAL:O	1:A:494:THR:HG23	2.05	0.57
1:A:301:SER:CB	1:A:452:ALA:HB3	2.35	0.56
1:C:17:PHE:HB3	1:C:131:LEU:HD13	1.87	0.56
1:D:184:SER:CA	1:D:246:GLU:HG3	2.23	0.56
1:B:725:LEU:O	1:B:725:LEU:HD23	2.05	0.56
1:C:127:SER:OG	1:C:305:ILE:HG21	2.05	0.56
1:D:168:ASN:OD1	1:D:524:PRO:HD3	2.05	0.56
1:D:280:LYS:O	1:D:284:GLN:HG3	2.04	0.56
1:A:10:ILE:N	1:A:11:PRO:HD2	2.19	0.56
1:C:293:PHE:CZ	1:C:336:THR:HG21	2.41	0.56
1:C:325:LEU:HD23	1:C:453:THR:CG2	2.34	0.56
1:C:402:THR:HG21	1:C:686:ILE:HG21	1.86	0.56
1:C:421:THR:O	1:C:425:VAL:HG23	2.05	0.56
1:D:704:ILE:O	1:D:708:ILE:HG22	2.05	0.56
1:B:112:THR:CG2	1:B:117:PRO:HG2	2.35	0.56
1:C:517:TYR:CB	1:C:714:VAL:HG22	2.28	0.56
1:D:39:SER:HA	1:D:42:ILE:HD11	1.86	0.56
1:D:573:MET:SD	1:D:603:THR:HG23	2.45	0.56
1:A:571:MET:HG3	1:B:404:MET:CE	2.36	0.56
1:B:8:PHE:HD1	1:B:142:VAL:CG2	2.18	0.56
1:B:448:LEU:CD1	1:B:505:SER:HB2	2.35	0.56
1:C:398:SER:HB3	1:C:684:LEU:HD21	1.87	0.56
1:D:194:GLY:O	1:D:198:THR:HG22	2.05	0.56
1:D:209:GLY:O	1:D:214:ASN:N	2.39	0.56
1:D:400:GLU:HB2	1:D:404:MET:HG3	1.85	0.56
1:C:321:LEU:HD13	1:C:457:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ILE:HD11	1:C:534:VAL:CG2	2.35	0.56
1:D:448:LEU:CD1	1:D:505:SER:HB3	2.35	0.56
1:A:248:PHE:O	1:A:252:ILE:HG13	2.05	0.56
1:B:60:VAL:O	1:B:64:ILE:HG12	2.06	0.56
1:B:101:ALA:O	1:B:105:VAL:HG23	2.06	0.56
1:B:280:LYS:O	1:B:284:GLN:HG3	2.06	0.56
1:C:596:TYR:O	1:C:600:ILE:HG12	2.05	0.56
1:D:126:GLY:O	1:D:456:SER:HA	2.06	0.56
1:A:169:PHE:HB2	1:A:174:MET:HE2	1.88	0.56
1:A:299:GLY:HA2	1:A:302:MET:CE	2.35	0.56
1:B:385:SER:HA	1:B:661:ASN:HD22	1.71	0.56
1:C:89:SER:O	1:C:93:VAL:HG23	2.06	0.56
1:C:337:ALA:HB2	1:C:363:TRP:CZ2	2.41	0.56
1:C:422:LEU:O	1:C:422:LEU:HD23	2.06	0.56
1:D:102:ASN:OD1	1:D:103:VAL:N	2.37	0.56
1:D:219:ASP:OD1	1:D:220:PRO:HD2	2.06	0.56
1:A:120:LYS:HG3	1:A:313:PRO:HB3	1.88	0.56
1:A:185:ILE:HD13	1:A:619:ILE:HD11	1.88	0.56
1:A:656:GLY:HA3	1:A:695:LYS:HB2	1.88	0.56
1:B:277:GLN:HB3	1:B:352:VAL:HG11	1.87	0.56
1:C:116:GLY:HA3	1:C:313:PRO:HB2	1.86	0.56
1:D:112:THR:HG21	1:D:117:PRO:HG2	1.87	0.56
1:A:84:ALA:CB	1:A:186:ILE:HG13	2.36	0.56
1:B:53:GLU:HG3	1:B:611:MET:SD	2.46	0.56
1:B:199:LYS:CD	1:B:696:ASP:HB2	2.36	0.56
1:B:219:ASP:OD1	1:B:220:PRO:HD2	2.06	0.56
1:B:247:SER:HA	1:B:707:LYS:HE3	1.88	0.56
1:C:103:VAL:HG22	1:C:470:ILE:HG21	1.88	0.56
1:C:213:LEU:CB	1:C:215:LEU:HD13	2.36	0.56
1:B:309:ILE:CD1	1:B:310:VAL:HG23	2.36	0.55
1:D:468:GLY:N	1:D:484:THR:HG21	2.20	0.55
1:A:176:VAL:HB	1:A:253:VAL:HG13	1.88	0.55
1:B:155:VAL:HG22	1:B:172:PHE:CD2	2.41	0.55
1:C:25:VAL:CG2	1:C:124:GLN:HB3	2.36	0.55
1:C:208:VAL:HG23	1:C:574:VAL:HG22	1.88	0.55
1:A:252:ILE:HG12	1:A:445:LEU:HD13	1.87	0.55
1:A:347:LEU:HD12	1:A:350:LEU:HD11	1.88	0.55
1:A:422:LEU:HD23	1:A:422:LEU:O	2.06	0.55
1:A:578:ARG:O	1:A:582:ARG:HG2	2.07	0.55
1:C:80:PHE:HE2	1:C:185:ILE:HD12	1.70	0.55
1:C:97:MET:CE	1:C:125:GLY:HA2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:MET:CE	1:C:241:GLY:HA3	2.37	0.55
1:C:240:LEU:HD12	1:C:244:LEU:HD13	1.88	0.55
1:D:53:GLU:O	1:D:57:ILE:HG23	2.05	0.55
1:A:11:PRO:O	1:A:15:LEU:HG	2.06	0.55
1:A:414:MET:HG2	1:A:651:LEU:CD1	2.36	0.55
1:B:11:PRO:O	1:B:15:LEU:HG	2.07	0.55
1:B:380:ALA:HB3	1:B:497:ILE:HG12	1.87	0.55
1:C:398:SER:HB2	1:C:684:LEU:HG	1.89	0.55
1:D:300:CYS:SG	1:D:335:LEU:HD22	2.46	0.55
1:D:710:SER:O	1:D:714:VAL:HG23	2.06	0.55
1:B:301:SER:HB3	1:B:452:ALA:HB3	1.88	0.55
1:C:244:LEU:HD23	1:C:455:VAL:CG2	2.31	0.55
1:A:421:THR:O	1:A:425:VAL:HG23	2.06	0.55
1:B:296:VAL:HG21	1:B:339:LEU:HD22	1.89	0.55
1:A:474:CYS:HB2	1:A:476:LEU:CD1	2.37	0.55
1:A:621:THR:HB	1:A:622:PRO:HD3	1.88	0.55
1:A:718:SER:O	1:A:721:LYS:HE2	2.07	0.55
1:B:384:THR:CG2	1:B:493:THR:HG23	2.37	0.55
1:B:563:ILE:O	1:B:567:THR:HG23	2.07	0.55
1:C:120:LYS:CG	1:C:313:PRO:HB3	2.37	0.55
1:C:356:ARG:HG3	1:C:357:PHE:CD1	2.42	0.55
1:C:522:ILE:HD11	1:C:534:VAL:HG22	1.89	0.55
1:D:109:ALA:HB2	1:D:118:ALA:HB2	1.89	0.55
1:D:126:GLY:HA2	1:D:459:SER:OG	2.07	0.55
1:D:543:ARG:HH22	1:D:726:PHE:C	2.10	0.55
1:D:725:LEU:HD23	1:D:725:LEU:O	2.07	0.55
1:A:155:VAL:HG22	1:A:172:PHE:CD2	2.42	0.55
1:A:194:GLY:HA3	1:A:235:GLY:HA2	1.89	0.55
1:A:563:ILE:O	1:A:567:THR:HG23	2.07	0.55
1:B:479:GLU:O	1:B:482:LYS:HG2	2.07	0.55
1:C:386:TYR:HD2	1:C:665:TYR:HD2	1.53	0.55
1:C:521:GLN:NE2	1:C:631:ALA:HB1	2.23	0.55
1:D:31:GLY:CA	1:D:107:GLU:HG3	2.34	0.55
1:A:21:ASN:HB2	1:A:128:VAL:HG22	1.88	0.54
1:C:219:ASP:OD1	1:C:220:PRO:HD2	2.06	0.54
1:C:286:LEU:HB3	1:C:438:TYR:HE2	1.72	0.54
1:D:363:TRP:CZ2	1:D:367:ILE:HD11	2.42	0.54
1:D:421:THR:O	1:D:425:VAL:HG23	2.08	0.54
1:A:309:ILE:HD12	1:A:310:VAL:HG23	1.89	0.54
1:A:666:LEU:CD1	1:A:684:LEU:HD12	2.37	0.54
1:C:218:ASP:HA	1:C:225:THR:CG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:ALA:HB1	1:C:708:ILE:CG2	2.38	0.54
1:B:167:ILE:HG13	1:B:719:ILE:HG13	1.89	0.54
1:B:291:ILE:O	1:B:295:LEU:HG	2.06	0.54
1:D:208:VAL:HG11	1:D:577:ILE:CG2	2.37	0.54
1:D:215:LEU:HD21	1:D:221:ARG:HB2	1.87	0.54
1:C:119:LEU:HD22	1:C:317:PRO:HA	1.88	0.54
1:C:204:ALA:HB3	1:C:573:MET:HE2	1.89	0.54
1:C:336:THR:HG22	1:C:363:TRP:CD1	2.40	0.54
1:C:517:TYR:HB2	1:C:714:VAL:CG2	2.30	0.54
1:B:110:ARG:HD3	1:B:476:LEU:HD23	1.90	0.54
1:B:718:SER:HA	1:B:721:LYS:CD	2.35	0.54
1:C:137:ALA:HB2	1:C:245:LEU:HG	1.89	0.54
1:C:678:SER:HB2	1:C:680:PRO:HD2	1.89	0.54
1:D:39:SER:O	1:D:43:ARG:HG3	2.08	0.54
1:A:57:ILE:HG12	1:A:189:PHE:HB3	1.88	0.54
1:B:117:PRO:O	1:B:121:VAL:HG12	2.08	0.54
1:D:141:LEU:CD2	1:D:252:ILE:HG21	2.37	0.54
1:D:506:ALA:HB2	1:D:707:LYS:NZ	2.23	0.54
1:A:219:ASP:OD1	1:A:220:PRO:HD2	2.06	0.54
1:B:32:THR:H	1:B:35:MET:CE	2.20	0.54
1:B:503:ILE:HD11	1:B:646:ALA:HA	1.90	0.54
1:D:14:ALA:HA	1:D:302:MET:SD	2.47	0.54
1:A:120:LYS:HZ1	1:A:309:ILE:HA	1.72	0.54
1:B:704:ILE:O	1:B:708:ILE:HG22	2.07	0.54
1:C:194:GLY:O	1:C:198:THR:HG22	2.08	0.54
1:C:340:THR:HG22	1:C:359:ALA:O	2.08	0.54
1:C:395:GLY:O	1:C:398:SER:OG	2.16	0.54
1:C:656:GLY:HA3	1:C:695:LYS:HB3	1.90	0.54
1:D:60:VAL:O	1:D:64:ILE:HG12	2.06	0.54
1:D:356:ARG:HD2	1:D:433:TYR:O	2.08	0.54
1:A:522:ILE:HD11	1:A:534:VAL:CG1	2.38	0.54
1:B:21:ASN:HB2	1:B:128:VAL:HG22	1.90	0.54
1:C:43:ARG:HG2	1:C:99:THR:CB	2.27	0.54
1:C:170:VAL:HB	1:C:173:ALA:HB3	1.88	0.54
1:A:377:GLY:CA	1:A:497:ILE:HG23	2.37	0.54
1:B:401:GLY:O	1:B:405:VAL:HG23	2.07	0.54
1:B:474:CYS:HB2	1:B:476:LEU:HD11	1.90	0.54
1:B:627:PHE:HE1	1:B:719:ILE:HG22	1.73	0.54
1:D:167:ILE:HD11	1:D:719:ILE:HD11	1.89	0.54
1:D:232:ASP:O	1:D:236:ASP:HB2	2.08	0.54
1:A:363:TRP:CE2	1:A:367:ILE:HD11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASP:OD1	1:A:526:ASP:N	2.37	0.53
1:B:248:PHE:O	1:B:252:ILE:HG13	2.08	0.53
1:C:188:MET:HE3	1:C:558:PHE:HZ	1.73	0.53
1:D:386:TYR:HD2	1:D:665:TYR:HD2	1.56	0.53
1:D:167:ILE:CG1	1:D:719:ILE:HD11	2.37	0.53
1:B:112:THR:HG21	1:B:117:PRO:CG	2.38	0.53
1:C:110:ARG:HA	1:C:480:VAL:HG22	1.90	0.53
1:C:115:ILE:HG13	1:C:483:ILE:HD12	1.90	0.53
1:D:222:ASN:HB3	1:D:225:THR:CG2	2.35	0.53
1:B:308:VAL:HG21	1:B:324:SER:CA	2.39	0.53
1:C:537:LEU:CD2	1:C:639:ILE:HD11	2.36	0.53
1:A:169:PHE:HB2	1:A:174:MET:CE	2.38	0.53
1:A:325:LEU:HD23	1:A:453:THR:CG2	2.36	0.53
1:A:448:LEU:O	1:A:451:VAL:HB	2.08	0.53
1:B:102:ASN:HB2	1:B:466:ASN:HB3	1.89	0.53
1:B:469:GLY:O	1:B:473:MET:HG3	2.08	0.53
1:B:615:ALA:O	1:B:619:ILE:HG13	2.09	0.53
1:C:409:GLY:HA3	1:C:659:TRP:CZ2	2.44	0.53
1:C:535:LEU:CA	1:D:540:LEU:HD22	2.38	0.53
1:D:703:ASP:OD1	1:D:704:ILE:HD12	2.09	0.53
1:A:363:TRP:CH2	1:A:367:ILE:HD11	2.44	0.53
1:B:112:THR:OG1	1:B:117:PRO:HG2	2.08	0.53
1:B:130:GLY:HA2	1:B:455:VAL:HB	1.89	0.53
1:B:213:LEU:CB	1:B:215:LEU:HD13	2.39	0.53
1:C:188:MET:HB2	1:C:704:ILE:HG21	1.90	0.53
1:D:355:PHE:HB3	1:D:361:SER:HB2	1.90	0.53
1:A:545:ILE:HG21	1:B:511:LEU:CD1	2.38	0.53
1:B:188:MET:HB2	1:B:704:ILE:HG21	1.90	0.53
1:B:293:PHE:CE2	1:B:336:THR:HG21	2.44	0.53
1:C:10:ILE:N	1:C:11:PRO:HD2	2.23	0.53
1:C:129:MET:HE1	1:C:241:GLY:N	2.22	0.53
1:D:47:ASP:OD1	1:D:95:MET:HE3	2.09	0.53
1:B:110:ARG:HD3	1:B:476:LEU:CD2	2.38	0.53
1:B:194:GLY:O	1:B:198:THR:HG22	2.09	0.53
1:C:370:ILE:O	1:C:374:ILE:HG13	2.08	0.53
1:C:386:TYR:CD2	1:C:665:TYR:HB2	2.44	0.53
1:C:399:ILE:HD11	1:C:671:LEU:CD2	2.33	0.53
1:D:547:GLY:O	1:D:637:VAL:HA	2.09	0.53
1:A:53:GLU:HG3	1:A:611:MET:CE	2.39	0.53
1:B:169:PHE:CB	1:B:174:MET:HE3	2.38	0.53
1:C:717:VAL:HA	1:C:720:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:CE2	1:B:182:GLY:HA2	2.44	0.53
1:C:398:SER:HA	1:C:405:VAL:HG22	1.90	0.53
1:C:584:ILE:CG2	1:C:587:LEU:HB2	2.38	0.53
1:D:10:ILE:N	1:D:11:PRO:HD2	2.24	0.53
1:B:218:ASP:HA	1:B:225:THR:CG2	2.38	0.52
1:B:248:PHE:CZ	1:B:294:ALA:HB1	2.44	0.52
1:C:160:ILE:O	1:C:160:ILE:CG2	2.57	0.52
1:D:141:LEU:HD21	1:D:252:ILE:CG2	2.39	0.52
1:D:493:THR:O	1:D:497:ILE:HG13	2.09	0.52
1:A:326:TRP:O	1:A:330:LEU:HD13	2.09	0.52
1:A:363:TRP:CZ2	1:A:367:ILE:HD11	2.44	0.52
1:B:119:LEU:HD22	1:B:317:PRO:HB3	1.91	0.52
1:B:725:LEU:HD22	1:B:726:PHE:CZ	2.44	0.52
1:D:149:GLY:HA2	1:D:155:VAL:HG23	1.92	0.52
1:D:422:LEU:HD23	1:D:422:LEU:O	2.08	0.52
1:A:53:GLU:HG2	1:A:57:ILE:HD11	1.91	0.52
1:B:422:LEU:O	1:B:422:LEU:HD23	2.09	0.52
1:C:84:ALA:HA	1:C:186:ILE:HG13	1.92	0.52
1:C:557:TYR:HD1	1:D:415:LYS:HA	1.73	0.52
1:C:562:LEU:HD13	1:C:697:THR:HG22	1.90	0.52
1:C:573:MET:SD	1:C:603:THR:HG23	2.49	0.52
1:D:170:VAL:HG13	1:D:171:PRO:HD2	1.92	0.52
1:D:674:TYR:HB3	1:D:678:SER:OG	2.10	0.52
1:A:53:GLU:HG2	1:A:57:ILE:CD1	2.39	0.52
1:B:84:ALA:HB1	1:B:186:ILE:HG13	1.90	0.52
1:B:619:ILE:HG12	1:B:708:ILE:HD11	1.91	0.52
1:C:213:LEU:HB2	1:C:215:LEU:HD13	1.91	0.52
1:D:199:LYS:CD	1:D:696:ASP:HB2	2.39	0.52
1:D:331:LEU:O	1:D:335:LEU:HD13	2.09	0.52
1:A:323:ILE:O	1:A:327:THR:HG23	2.10	0.52
1:A:584:ILE:HG22	1:A:587:LEU:HB2	1.91	0.52
1:C:400:GLU:HG3	1:D:571:MET:HG2	1.90	0.52
1:D:293:PHE:CE2	1:D:336:THR:HG21	2.44	0.52
1:D:398:SER:HA	1:D:405:VAL:CG2	2.39	0.52
1:A:291:ILE:O	1:A:295:LEU:HG	2.09	0.52
1:A:300:CYS:SG	1:A:335:LEU:HD22	2.50	0.52
1:B:363:TRP:CZ3	1:B:367:ILE:HD11	2.44	0.52
1:C:119:LEU:HD13	1:C:317:PRO:HB3	1.91	0.52
1:C:226:ILE:HD12	1:C:596:TYR:CD2	2.45	0.52
1:A:384:THR:HG21	1:A:493:THR:HA	1.92	0.52
1:B:410:LEU:O	1:B:414:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:LEU:HD22	1:C:726:PHE:CE1	2.45	0.52
1:D:101:ALA:O	1:D:105:VAL:HG23	2.10	0.52
1:D:184:SER:HA	1:D:246:GLU:CG	2.26	0.52
1:D:479:GLU:O	1:D:482:LYS:HG2	2.10	0.52
1:B:573:MET:SD	1:B:603:THR:HG23	2.49	0.52
1:D:261:TYR:O	1:D:265:ILE:HD13	2.10	0.52
1:A:57:ILE:HG22	1:A:186:ILE:HD12	1.91	0.52
1:A:187:ALA:HA	1:A:242:ALA:HB1	1.92	0.52
1:B:208:VAL:HG21	1:B:574:VAL:HA	1.92	0.52
1:B:652:THR:HB	1:B:694:LEU:O	2.10	0.52
1:D:622:PRO:HB3	1:D:713:SER:OG	2.09	0.52
1:A:322:ASN:HD22	1:A:322:ASN:N	2.08	0.52
1:B:127:SER:OG	1:B:305:ILE:HG21	2.10	0.52
1:B:133:VAL:HG13	1:B:245:LEU:HB2	1.92	0.52
1:C:208:VAL:HG11	1:C:577:ILE:CG2	2.39	0.52
1:D:291:ILE:O	1:D:295:LEU:HG	2.09	0.52
1:D:598:ARG:O	1:D:602:ILE:HG12	2.10	0.52
1:A:399:ILE:CD1	1:A:671:LEU:HD21	2.35	0.51
1:B:300:CYS:SG	1:B:332:THR:HA	2.50	0.51
1:C:573:MET:O	1:C:577:ILE:HG13	2.10	0.51
1:D:223:PRO:HB3	1:D:580:GLN:HE22	1.75	0.51
1:D:258:LEU:HD23	1:D:262:MET:HG3	1.92	0.51
1:D:323:ILE:O	1:D:327:THR:HG23	2.11	0.51
1:D:424:LEU:HD23	1:D:507:ILE:HD12	1.92	0.51
1:D:681:HIS:O	1:D:685:VAL:HG23	2.10	0.51
1:A:194:GLY:O	1:A:198:THR:HG22	2.10	0.51
1:A:390:PRO:HB2	1:A:412:LEU:HD11	1.91	0.51
1:B:42:ILE:HD12	1:B:226:ILE:HG23	1.90	0.51
1:B:266:TYR:CD1	1:B:531:PRO:HG2	2.45	0.51
1:B:629:LEU:HD23	1:B:726:PHE:HD2	1.75	0.51
1:C:69:MET:CE	1:C:74:TRP:HB2	2.40	0.51
1:C:545:ILE:HD13	1:D:511:LEU:HG	1.93	0.51
1:A:266:TYR:CE1	1:A:531:PRO:HG2	2.45	0.51
1:A:596:TYR:O	1:A:600:ILE:HG12	2.10	0.51
1:B:115:ILE:HG23	1:B:487:LEU:HD21	1.91	0.51
1:B:232:ASP:O	1:B:236:ASP:HB2	2.10	0.51
1:D:652:THR:HB	1:D:694:LEU:O	2.10	0.51
1:A:60:VAL:O	1:A:64:ILE:HG13	2.11	0.51
1:A:145:TYR:OH	1:A:288:SER:OG	2.23	0.51
1:A:177:SER:CB	1:A:715:ILE:HD11	2.40	0.51
1:B:189:PHE:CE1	1:B:612:GLY:HA2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:PHE:HZ	1:D:294:ALA:HB1	1.75	0.51
1:B:41:TYR:CD2	1:B:226:ILE:HD13	2.45	0.51
1:B:660:ASP:O	1:B:664:LYS:HG3	2.11	0.51
1:C:102:ASN:HB2	1:C:466:ASN:HB3	1.92	0.51
1:C:248:PHE:O	1:C:252:ILE:HG13	2.11	0.51
1:C:288:SER:HB2	1:C:343:TYR:OH	2.11	0.51
1:C:291:ILE:O	1:C:295:LEU:HG	2.10	0.51
1:C:710:SER:O	1:C:714:VAL:HG23	2.11	0.51
1:A:370:ILE:HG23	1:A:450:PHE:HE2	1.75	0.51
1:B:47:ASP:OD1	1:B:95:MET:HE3	2.10	0.51
1:B:53:GLU:O	1:B:57:ILE:HG23	2.11	0.51
1:B:561:TYR:HH	1:B:613:TYR:HD2	1.57	0.51
1:C:60:VAL:O	1:C:64:ILE:HG12	2.10	0.51
1:A:337:ALA:HB2	1:A:363:TRP:CZ2	2.45	0.51
1:A:627:PHE:HE1	1:A:719:ILE:HG22	1.76	0.51
1:C:622:PRO:HG3	1:C:709:MET:CG	2.31	0.51
1:D:321:LEU:HD13	1:D:457:VAL:HG13	1.91	0.51
1:A:110:ARG:HA	1:A:480:VAL:HG22	1.92	0.51
1:B:78:VAL:HG21	1:B:148:PHE:CZ	2.45	0.51
1:C:301:SER:HB3	1:C:452:ALA:HB3	1.91	0.51
1:D:500:GLY:O	1:D:503:ILE:HG22	2.10	0.51
1:A:399:ILE:HD12	1:A:674:TYR:CE2	2.46	0.51
1:A:553:ALA:HB2	1:B:421:THR:CG2	2.36	0.51
1:B:107:GLU:O	1:B:111:THR:HG23	2.11	0.51
1:B:159:ASN:HB2	1:B:161:TYR:CE1	2.46	0.51
1:B:386:TYR:HD2	1:B:665:TYR:HD1	1.59	0.51
1:B:710:SER:O	1:B:714:VAL:HG23	2.11	0.51
1:C:133:VAL:HG13	1:C:245:LEU:HB2	1.93	0.51
1:C:227:ALA:HA	1:C:600:ILE:CD1	2.41	0.51
1:C:377:GLY:HA2	1:C:497:ILE:HG23	1.93	0.51
1:C:399:ILE:CD1	1:C:671:LEU:HD21	2.32	0.51
1:C:618:ALA:HB1	1:C:708:ILE:HG21	1.92	0.51
1:D:207:LEU:O	1:D:211:THR:HB	2.11	0.51
1:D:249:VAL:O	1:D:253:VAL:HG23	2.11	0.51
1:D:395:GLY:O	1:D:398:SER:OG	2.15	0.51
1:B:169:PHE:HB2	1:B:174:MET:CE	2.42	0.51
1:C:621:THR:HB	1:C:622:PRO:HD3	1.93	0.51
1:D:167:ILE:HG12	1:D:719:ILE:CG1	2.41	0.51
1:D:176:VAL:HB	1:D:253:VAL:HG13	1.91	0.51
1:D:208:VAL:HG11	1:D:577:ILE:HG22	1.93	0.51
1:D:627:PHE:CE1	1:D:720:PHE:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:O	1:A:587:LEU:HD21	2.11	0.50
1:B:23:ALA:HA	1:B:26:VAL:HG12	1.93	0.50
1:B:38:ILE:HD12	1:B:474:CYS:SG	2.51	0.50
1:D:38:ILE:O	1:D:42:ILE:HG12	2.11	0.50
1:D:159:ASN:HB3	1:D:161:TYR:CE1	2.46	0.50
1:A:216:PRO:HG2	1:A:219:ASP:HB2	1.93	0.50
1:A:280:LYS:O	1:A:284:GLN:HG3	2.11	0.50
1:A:666:LEU:HD13	1:A:684:LEU:HD12	1.93	0.50
1:B:54:THR:O	1:B:57:ILE:HG13	2.10	0.50
1:B:648:LEU:O	1:B:652:THR:HG23	2.12	0.50
1:C:285:ALA:HB3	1:C:347:LEU:HD13	1.93	0.50
1:C:557:TYR:CD1	1:D:415:LYS:HA	2.46	0.50
1:C:718:SER:O	1:C:721:LYS:HE2	2.11	0.50
1:A:7:PHE:O	1:A:295:LEU:HD13	2.12	0.50
1:A:223:PRO:HA	1:A:596:TYR:CD1	2.46	0.50
1:B:119:LEU:HD13	1:B:317:PRO:HB3	1.92	0.50
1:D:89:SER:O	1:D:93:VAL:HG23	2.12	0.50
1:D:263:PHE:HB2	1:D:283:ILE:HG13	1.92	0.50
1:A:217:GLU:O	1:A:472:GLU:HG2	2.11	0.50
1:A:223:PRO:HG2	1:A:577:ILE:HG12	1.92	0.50
1:A:386:TYR:HD1	1:A:386:TYR:H	1.60	0.50
1:B:25:VAL:HG11	1:B:97:MET:HE1	1.92	0.50
1:B:165:LEU:HB3	1:B:167:ILE:HD13	1.94	0.50
1:B:233:ASN:OD1	1:B:466:ASN:ND2	2.44	0.50
1:C:545:ILE:HD13	1:D:511:LEU:CG	2.42	0.50
1:D:192:VAL:HG11	1:D:614:PRO:HG3	1.92	0.50
1:D:384:THR:CG2	1:D:493:THR:HG23	2.41	0.50
1:D:678:SER:HB2	1:D:680:PRO:HD2	1.94	0.50
1:A:47:ASP:OD1	1:A:95:MET:HE3	2.11	0.50
1:A:308:VAL:HG21	1:A:324:SER:CB	2.28	0.50
1:A:402:THR:HG21	1:A:686:ILE:HG21	1.93	0.50
1:B:372:SER:O	1:B:376:ILE:HG13	2.11	0.50
1:B:390:PRO:HB2	1:B:412:LEU:HD11	1.92	0.50
1:C:437:LEU:HD13	1:C:515:ALA:CB	2.41	0.50
1:C:459:SER:O	1:C:462:PRO:HD2	2.11	0.50
1:A:35:MET:HE1	1:A:476:LEU:HD21	1.94	0.50
1:A:133:VAL:HG13	1:A:245:LEU:HB2	1.92	0.50
1:A:477:ASP:OD1	1:A:478:PRO:HD2	2.12	0.50
1:B:187:ALA:HA	1:B:242:ALA:HB1	1.92	0.50
1:C:308:VAL:CG2	1:C:324:SER:HB2	2.17	0.50
1:C:340:THR:HG21	1:C:362:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:GLN:HG2	1:C:717:VAL:CG2	2.42	0.50
1:D:563:ILE:HD11	1:D:694:LEU:CD2	2.42	0.50
1:A:167:ILE:CD1	1:A:719:ILE:HD11	2.35	0.50
1:A:507:ILE:HD11	1:A:646:ALA:HB2	1.93	0.50
1:B:386:TYR:HA	1:B:391:THR:HB	1.94	0.50
1:B:621:THR:HB	1:B:622:PRO:HD3	1.92	0.50
1:D:30:GLU:O	1:D:107:GLU:HG3	2.11	0.50
1:D:84:ALA:CA	1:D:186:ILE:HG13	2.41	0.50
1:D:405:VAL:HG11	1:D:684:LEU:HD23	1.93	0.50
1:D:471:SER:HB2	1:D:476:LEU:HD22	1.94	0.50
1:A:402:THR:HB	1:B:686:ILE:HD13	1.92	0.50
1:A:471:SER:O	1:A:476:LEU:HD13	2.12	0.50
1:B:84:ALA:CA	1:B:186:ILE:HG13	2.41	0.50
1:B:88:ALA:O	1:B:92:ILE:HG13	2.12	0.50
1:B:168:ASN:OD1	1:B:721:LYS:HE2	2.11	0.50
1:C:115:ILE:HB	1:C:315:ASP:HA	1.92	0.50
1:A:84:ALA:HB1	1:A:186:ILE:HG13	1.94	0.50
1:A:622:PRO:CG	1:A:709:MET:HG3	2.35	0.50
1:B:61:ALA:HB2	1:B:186:ILE:HD11	1.94	0.50
1:B:267:VAL:HG12	1:B:276:HIS:HA	1.94	0.50
1:B:402:THR:HG21	1:B:686:ILE:HG21	1.93	0.50
1:B:517:TYR:CB	1:B:714:VAL:HG22	2.33	0.50
1:C:138:LEU:HD21	1:C:294:ALA:HB1	1.94	0.50
1:D:129:MET:HE1	1:D:241:GLY:H	1.76	0.50
1:D:88:ALA:O	1:D:92:ILE:HG13	2.12	0.49
1:D:615:ALA:O	1:D:619:ILE:HG13	2.12	0.49
1:A:356:ARG:HD2	1:A:433:TYR:O	2.12	0.49
1:A:547:GLY:O	1:A:637:VAL:HA	2.12	0.49
1:B:199:LYS:HD2	1:B:692:ASP:O	2.12	0.49
1:B:306:LEU:HD12	1:B:309:ILE:HD11	1.95	0.49
1:C:468:GLY:HA2	1:C:484:THR:HG21	1.94	0.49
1:C:627:PHE:CE1	1:C:720:PHE:HB3	2.48	0.49
1:D:160:ILE:CG2	1:D:527:ILE:HD12	2.42	0.49
1:D:460:TYR:HE2	1:D:490:VAL:HG12	1.76	0.49
1:A:263:PHE:HB3	1:A:264:PRO:HD3	1.95	0.49
1:B:89:SER:O	1:B:93:VAL:HG23	2.12	0.49
1:B:107:GLU:OE2	1:B:111:THR:HG21	2.13	0.49
1:C:84:ALA:CA	1:C:186:ILE:HG13	2.41	0.49
1:C:581:ALA:HB1	1:C:588:LEU:HD11	1.94	0.49
1:D:138:LEU:HD12	1:D:298:LEU:CD1	2.42	0.49
1:A:309:ILE:CD1	1:A:310:VAL:HG23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:MET:HG2	1:A:651:LEU:HD12	1.94	0.49
1:B:105:VAL:CG2	1:B:121:VAL:HG22	2.42	0.49
1:B:218:ASP:HA	1:B:225:THR:HG22	1.95	0.49
1:B:363:TRP:CH2	1:B:367:ILE:HD11	2.47	0.49
1:B:419:PRO:N	1:B:420:PRO:HD2	2.28	0.49
1:A:192:VAL:HG11	1:A:614:PRO:CG	2.38	0.49
1:A:401:GLY:O	1:A:405:VAL:HG23	2.12	0.49
1:A:493:THR:O	1:A:497:ILE:HG13	2.12	0.49
1:A:527:ILE:O	1:A:527:ILE:HG12	2.12	0.49
1:B:32:THR:OG1	1:B:33:GLU:N	2.44	0.49
1:D:613:TYR:N	1:D:614:PRO:HD2	2.27	0.49
1:D:621:THR:HB	1:D:622:PRO:HD3	1.94	0.49
1:A:82:LEU:HD23	1:A:144:VAL:HG23	1.94	0.49
1:A:363:TRP:CZ3	1:A:367:ILE:HD11	2.48	0.49
1:B:160:ILE:CG2	1:B:527:ILE:HD12	2.42	0.49
1:B:566:VAL:HG11	1:B:693:PRO:HB3	1.93	0.49
1:C:410:LEU:O	1:C:414:MET:HG3	2.12	0.49
1:D:155:VAL:O	1:D:155:VAL:HG12	2.13	0.49
1:A:347:LEU:HB2	1:A:350:LEU:HD11	1.94	0.49
1:B:377:GLY:HA2	1:B:497:ILE:HG23	1.95	0.49
1:B:514:PHE:CE1	1:B:638:LEU:HB3	2.46	0.49
1:D:409:GLY:HA3	1:D:659:TRP:CZ2	2.48	0.49
1:A:149:GLY:HA2	1:A:155:VAL:HG23	1.93	0.49
1:A:580:GLN:NE2	1:A:595:ASP:HB3	2.28	0.49
1:A:647:MET:HG3	1:B:552:ALA:HB1	1.94	0.49
1:B:226:ILE:O	1:B:230:VAL:HG23	2.13	0.49
1:B:437:LEU:H	1:B:437:LEU:HD22	1.78	0.49
1:C:109:ALA:HB2	1:C:118:ALA:HB2	1.95	0.49
1:C:535:LEU:HD22	1:D:540:LEU:HD23	1.95	0.49
1:D:97:MET:CE	1:D:125:GLY:HA2	2.42	0.49
1:D:561:TYR:HE2	1:D:614:PRO:HD3	1.78	0.49
1:A:553:ALA:CB	1:B:421:THR:HG21	2.36	0.49
1:A:667:GLU:HG2	1:A:681:HIS:NE2	2.28	0.49
1:B:97:MET:CE	1:B:125:GLY:HA2	2.43	0.49
1:B:278:VAL:HG11	1:B:353:LEU:CD2	2.43	0.49
1:C:419:PRO:N	1:C:420:PRO:HD2	2.28	0.49
1:C:547:GLY:O	1:C:637:VAL:HA	2.12	0.49
1:D:7:PHE:O	1:D:10:ILE:HG13	2.12	0.49
1:A:208:VAL:HG23	1:A:574:VAL:HG22	1.95	0.49
1:A:372:SER:HB2	1:A:447:MET:HE2	1.93	0.49
1:B:249:VAL:O	1:B:253:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:SER:O	1:B:476:LEU:HD13	2.12	0.49
1:B:522:ILE:HD11	1:B:534:VAL:CG1	2.42	0.49
1:B:678:SER:HB2	1:B:680:PRO:HD2	1.95	0.49
1:C:102:ASN:CB	1:C:466:ASN:HB3	2.43	0.49
1:C:115:ILE:HG21	1:C:317:PRO:HD3	1.95	0.49
1:A:474:CYS:HB2	1:A:476:LEU:HD11	1.95	0.48
1:B:102:ASN:CB	1:B:466:ASN:HB3	2.43	0.48
1:B:301:SER:OG	1:B:450:PHE:HA	2.12	0.48
1:C:97:MET:HE3	1:C:125:GLY:HA2	1.95	0.48
1:C:112:THR:OG1	1:C:117:PRO:HG2	2.13	0.48
1:C:389:LYS:N	1:C:390:PRO:HD2	2.28	0.48
1:D:124:GLN:O	1:D:128:VAL:HG23	2.13	0.48
1:D:363:TRP:CD2	1:D:367:ILE:HD11	2.48	0.48
1:A:75:GLN:HB3	1:A:148:PHE:CD2	2.48	0.48
1:B:399:ILE:CD1	1:B:671:LEU:HD21	2.40	0.48
1:C:188:MET:HB2	1:C:704:ILE:CG2	2.44	0.48
1:C:373:GLY:HA3	1:C:447:MET:HG3	1.94	0.48
1:C:535:LEU:HB3	1:D:540:LEU:CD2	2.43	0.48
1:A:678:SER:HB2	1:A:680:PRO:HD2	1.95	0.48
1:C:119:LEU:HD13	1:C:317:PRO:CB	2.43	0.48
1:C:248:PHE:CZ	1:C:252:ILE:HD11	2.49	0.48
1:C:280:LYS:O	1:C:284:GLN:HG3	2.13	0.48
1:D:57:ILE:CD1	1:D:186:ILE:HD12	2.41	0.48
1:D:474:CYS:HB2	1:D:476:LEU:HD11	1.95	0.48
1:A:57:ILE:HD11	1:A:611:MET:HE1	1.95	0.48
1:A:676:LYS:O	1:A:681:HIS:ND1	2.47	0.48
1:A:723:VAL:O	1:A:723:VAL:HG12	2.13	0.48
1:B:400:GLU:HB2	1:B:404:MET:HG3	1.94	0.48
1:C:248:PHE:HZ	1:C:294:ALA:HB1	1.78	0.48
1:C:493:THR:O	1:C:497:ILE:HG13	2.14	0.48
1:D:17:PHE:HB3	1:D:131:LEU:HD13	1.95	0.48
1:A:643:LEU:HD12	1:B:643:LEU:HD12	1.95	0.48
1:B:184:SER:HA	1:B:246:GLU:CG	2.31	0.48
1:B:569:ALA:HB2	1:B:606:ASN:OD1	2.14	0.48
1:C:698:VAL:HG12	1:C:702:LEU:HD11	1.96	0.48
1:D:97:MET:HE2	1:D:125:GLY:HA2	1.96	0.48
1:A:184:SER:CA	1:A:246:GLU:HG3	2.35	0.48
1:A:355:PHE:HB3	1:A:361:SER:HB2	1.96	0.48
1:A:529:LYS:HD3	1:A:529:LYS:HA	1.50	0.48
1:A:549:LEU:HD11	1:B:507:ILE:HG21	1.96	0.48
1:A:698:VAL:O	1:A:702:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:HD1	1:B:142:VAL:HG21	1.78	0.48
1:B:105:VAL:HG22	1:B:121:VAL:CG2	2.42	0.48
1:A:224:ALA:CB	1:A:577:ILE:HD11	2.43	0.48
1:B:188:MET:HB2	1:B:704:ILE:CG2	2.44	0.48
1:C:42:ILE:HD13	1:C:229:ASN:HB3	1.96	0.48
1:C:404:MET:CE	1:D:571:MET:HG3	2.43	0.48
1:D:305:ILE:O	1:D:309:ILE:HG12	2.14	0.48
1:A:705:LEU:HD23	1:A:705:LEU:C	2.34	0.48
1:B:477:ASP:OD1	1:B:478:PRO:HD2	2.13	0.48
1:C:155:VAL:O	1:C:155:VAL:HG12	2.14	0.48
1:A:363:TRP:CD2	1:A:367:ILE:HD11	2.49	0.48
1:B:194:GLY:HA3	1:B:235:GLY:HA2	1.95	0.48
1:C:222:ASN:HB3	1:C:225:THR:CG2	2.41	0.48
1:C:521:GLN:HG2	1:C:717:VAL:HG21	1.95	0.48
1:D:569:ALA:HB2	1:D:606:ASN:ND2	2.29	0.48
1:A:100:ARG:O	1:A:104:ARG:HG2	2.13	0.48
1:A:460:TYR:OH	1:A:487:LEU:HD22	2.13	0.48
1:B:25:VAL:CB	1:B:97:MET:HE1	2.44	0.48
1:D:441:ALA:HB2	1:D:512:SER:OG	2.13	0.48
1:A:471:SER:CA	1:A:476:LEU:HD13	2.42	0.47
1:A:648:LEU:O	1:A:652:THR:HG23	2.14	0.47
1:B:32:THR:H	1:B:35:MET:HE2	1.79	0.47
1:B:325:LEU:HD23	1:B:453:THR:HG22	1.95	0.47
1:C:386:TYR:HA	1:C:391:THR:HB	1.95	0.47
1:B:384:THR:HG21	1:B:493:THR:HA	1.95	0.47
1:B:584:ILE:HG23	1:B:584:ILE:O	2.14	0.47
1:A:337:ALA:HB2	1:A:363:TRP:CE2	2.49	0.47
1:A:613:TYR:N	1:A:614:PRO:HD2	2.28	0.47
1:B:22:PHE:O	1:B:26:VAL:HG12	2.14	0.47
1:B:547:GLY:O	1:B:637:VAL:HA	2.13	0.47
1:C:181:LEU:O	1:C:185:ILE:HG13	2.15	0.47
1:C:418:PHE:HB3	1:C:419:PRO:CD	2.41	0.47
1:C:578:ARG:O	1:C:582:ARG:HG2	2.14	0.47
1:D:244:LEU:HD23	1:D:455:VAL:CG2	2.33	0.47
1:A:262:MET:SD	1:A:353:LEU:HD22	2.55	0.47
1:B:630:GLY:HA2	1:B:724:HIS:HB3	1.96	0.47
1:C:249:VAL:O	1:C:253:VAL:HG23	2.15	0.47
1:C:264:PRO:O	1:C:527:ILE:HD11	2.14	0.47
1:C:421:THR:CG2	1:D:553:ALA:HB2	2.43	0.47
1:D:115:ILE:N	1:D:115:ILE:HD12	2.30	0.47
1:D:419:PRO:N	1:D:420:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:CD2	1:A:252:ILE:HG21	2.44	0.47
1:A:268:GLN:HG2	6:A:809:GQB:C10	2.44	0.47
1:A:571:MET:HG3	1:B:404:MET:HE1	1.96	0.47
1:B:613:TYR:N	1:B:614:PRO:HD2	2.29	0.47
1:D:105:VAL:HA	1:D:121:VAL:HG11	1.96	0.47
1:D:138:LEU:HD21	1:D:294:ALA:CB	2.44	0.47
1:D:581:ALA:HA	1:D:587:LEU:HD13	1.97	0.47
1:D:633:PHE:O	1:D:637:VAL:HG23	2.14	0.47
1:A:54:THR:HG22	1:A:58:PHE:HD2	1.80	0.47
1:A:155:VAL:O	1:A:155:VAL:HG12	2.14	0.47
1:B:11:PRO:HB2	1:B:139:LEU:HB2	1.96	0.47
1:C:129:MET:HE2	1:C:241:GLY:HA3	1.95	0.47
1:C:326:TRP:O	1:C:330:LEU:HD13	2.15	0.47
1:D:147:ILE:O	1:D:151:TRP:HB3	2.15	0.47
1:A:7:PHE:C	1:A:295:LEU:HD13	2.35	0.47
1:A:192:VAL:O	1:A:196:VAL:HG23	2.15	0.47
1:A:226:ILE:O	1:A:230:VAL:HG23	2.14	0.47
1:A:356:ARG:HG3	1:A:357:PHE:CD1	2.50	0.47
1:B:10:ILE:N	1:B:11:PRO:HD2	2.30	0.47
1:B:227:ALA:HA	1:B:600:ILE:CD1	2.44	0.47
1:B:385:SER:HA	1:B:661:ASN:ND2	2.30	0.47
1:B:722:HIS:CD2	1:B:723:VAL:HG23	2.49	0.47
1:C:112:THR:HG21	1:C:117:PRO:HG2	1.97	0.47
1:C:305:ILE:O	1:C:309:ILE:HG12	2.15	0.47
1:C:579:ARG:NH1	1:C:583:GLU:OE1	2.47	0.47
1:D:198:THR:HB	1:D:231:GLY:O	2.14	0.47
1:D:414:MET:HG2	1:D:651:LEU:HD11	1.96	0.47
1:D:616:PHE:O	1:D:620:LEU:HG	2.14	0.47
1:A:459:SER:O	1:A:462:PRO:HD2	2.15	0.47
1:A:550:LEU:O	1:A:554:ILE:HG13	2.15	0.47
1:B:54:THR:HG22	1:B:58:PHE:HD2	1.79	0.47
1:B:80:PHE:HE2	1:B:185:ILE:HD12	1.80	0.47
1:D:248:PHE:O	1:D:252:ILE:HG13	2.15	0.47
1:D:410:LEU:O	1:D:414:MET:HG3	2.15	0.47
1:A:685:VAL:O	1:A:689:THR:HG23	2.15	0.47
1:B:141:LEU:HD21	1:B:252:ILE:HG21	1.97	0.47
1:B:355:PHE:CD1	1:B:362:PRO:HD3	2.50	0.47
1:C:32:THR:OG1	1:C:33:GLU:N	2.47	0.47
1:C:43:ARG:CG	1:C:99:THR:HB	2.31	0.47
1:C:105:VAL:HG22	1:C:121:VAL:HG22	1.96	0.47
1:C:167:ILE:CD1	1:C:719:ILE:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:TRP:CD2	1:C:367:ILE:HD11	2.49	0.47
1:D:25:VAL:CG2	1:D:124:GLN:HB3	2.45	0.47
1:D:240:LEU:HD12	1:D:244:LEU:HD13	1.96	0.47
1:B:18:ALA:HB2	1:B:131:LEU:HB2	1.97	0.47
1:B:398:SER:HA	1:B:405:VAL:HG22	1.97	0.47
1:C:248:PHE:CZ	1:C:294:ALA:HB1	2.50	0.47
1:C:418:PHE:HA	1:D:553:ALA:HB1	1.97	0.47
1:C:553:ALA:HB2	1:D:421:THR:CG2	2.41	0.47
1:D:112:THR:CG2	1:D:117:PRO:HG2	2.45	0.47
1:D:504:GLY:O	1:D:508:PHE:HD1	1.98	0.47
1:D:692:ASP:HA	1:D:695:LYS:HE3	1.96	0.47
1:A:184:SER:O	1:A:708:ILE:HD11	2.15	0.46
1:B:323:ILE:O	1:B:327:THR:HG23	2.15	0.46
1:B:511:LEU:O	1:B:511:LEU:HD23	2.15	0.46
1:C:66:ILE:O	1:C:70:ILE:HG13	2.15	0.46
1:C:205:ALA:HB2	1:C:224:ALA:HB3	1.96	0.46
1:C:597:ASN:ND2	7:C:807:D1D:H1C1	2.31	0.46
1:D:167:ILE:HG12	1:D:719:ILE:HG13	1.96	0.46
1:D:233:ASN:OD1	1:D:466:ASN:ND2	2.48	0.46
1:A:80:PHE:HE2	1:A:185:ILE:HD12	1.81	0.46
1:B:17:PHE:HB3	1:B:131:LEU:HD13	1.96	0.46
1:B:493:THR:O	1:B:497:ILE:HG13	2.15	0.46
1:C:119:LEU:HD21	1:C:320:GLU:CG	2.45	0.46
1:C:226:ILE:O	1:C:230:VAL:HG23	2.15	0.46
1:C:296:VAL:HG11	1:C:335:LEU:HB3	1.96	0.46
1:D:119:LEU:HD22	1:D:317:PRO:HB3	1.97	0.46
1:B:70:ILE:HG22	1:B:71:PHE:CD1	2.51	0.46
1:B:155:VAL:O	1:B:155:VAL:HG12	2.14	0.46
1:B:208:VAL:HG11	1:B:577:ILE:HG22	1.96	0.46
1:C:616:PHE:O	1:C:620:LEU:HG	2.15	0.46
1:D:162:THR:HA	1:D:167:ILE:O	2.15	0.46
1:D:401:GLY:O	1:D:405:VAL:HG23	2.15	0.46
1:A:21:ASN:CB	1:A:128:VAL:HG22	2.45	0.46
1:C:119:LEU:CD2	1:C:317:PRO:HA	2.46	0.46
1:C:188:MET:HE3	1:C:558:PHE:CZ	2.51	0.46
1:C:402:THR:CG2	1:C:686:ILE:HG21	2.46	0.46
1:C:477:ASP:OD1	1:C:478:PRO:HD2	2.14	0.46
1:A:25:VAL:HG21	1:A:97:MET:CE	2.45	0.46
1:B:180:ALA:HB2	1:B:253:VAL:HG21	1.98	0.46
1:B:424:LEU:HD21	1:B:504:GLY:HA2	1.98	0.46
1:C:571:MET:HG2	1:D:400:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LEU:HA	1:D:142:VAL:HG12	1.97	0.46
1:D:215:LEU:CD2	1:D:221:ARG:HB2	2.46	0.46
1:D:626:GLY:HA2	1:D:630:GLY:O	2.15	0.46
1:D:705:LEU:HD23	1:D:705:LEU:C	2.35	0.46
1:A:170:VAL:HB	1:A:173:ALA:HB3	1.97	0.46
1:C:62:ILE:O	1:C:66:ILE:HG12	2.14	0.46
1:C:511:LEU:CD1	1:D:545:ILE:HG21	2.46	0.46
1:D:199:LYS:HE2	1:D:199:LYS:CA	2.44	0.46
1:D:363:TRP:CH2	1:D:367:ILE:HD11	2.51	0.46
1:A:109:ALA:HB2	1:A:118:ALA:CB	2.45	0.46
1:B:5:ALA:O	1:B:9:LEU:HD13	2.15	0.46
1:B:268:GLN:HG3	1:B:277:GLN:CG	2.45	0.46
1:C:205:ALA:HB2	1:C:224:ALA:CB	2.46	0.46
1:A:115:ILE:N	1:A:115:ILE:HD12	2.31	0.46
1:A:296:VAL:HG11	1:A:335:LEU:HB3	1.98	0.46
1:A:381:GLU:HG3	1:A:493:THR:HG21	1.97	0.46
1:A:571:MET:HG2	1:B:400:GLU:HG3	1.98	0.46
1:B:160:ILE:HG21	1:B:527:ILE:HD12	1.98	0.46
1:C:208:VAL:CG2	1:C:574:VAL:HG13	2.44	0.46
1:D:32:THR:OG1	1:D:33:GLU:N	2.49	0.46
1:D:103:VAL:HG22	1:D:470:ILE:HG21	1.97	0.46
1:A:32:THR:HG23	1:A:35:MET:H	1.81	0.46
1:A:386:TYR:HD2	1:A:665:TYR:HD2	1.62	0.46
1:A:419:PRO:N	1:A:420:PRO:HD2	2.31	0.46
1:B:651:LEU:HD23	1:B:651:LEU:C	2.36	0.46
1:C:549:LEU:HD11	1:D:507:ILE:HG21	1.98	0.46
1:D:723:VAL:O	1:D:723:VAL:HG12	2.16	0.46
1:A:25:VAL:CG2	1:A:97:MET:HE1	2.45	0.46
1:A:418:PHE:HB3	1:A:419:PRO:CD	2.42	0.46
1:B:301:SER:O	1:B:305:ILE:HG13	2.15	0.46
1:B:550:LEU:O	1:B:554:ILE:HG13	2.16	0.46
1:C:154:GLN:HB3	1:C:171:PRO:HB2	1.98	0.46
1:D:521:GLN:HG2	1:D:717:VAL:CG2	2.46	0.46
1:D:698:VAL:O	1:D:702:LEU:HG	2.15	0.46
1:C:514:PHE:CZ	1:C:642:VAL:HG21	2.51	0.45
1:C:527:ILE:HG23	1:C:527:ILE:O	2.15	0.45
1:D:550:LEU:O	1:D:554:ILE:HG13	2.16	0.45
1:A:11:PRO:HD3	1:A:295:LEU:CD2	2.46	0.45
1:A:615:ALA:O	1:A:619:ILE:HG13	2.15	0.45
1:C:25:VAL:HG21	1:C:97:MET:CE	2.47	0.45
1:A:301:SER:O	1:A:305:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ALA:O	1:A:574:VAL:HG23	2.16	0.45
1:B:115:ILE:N	1:B:115:ILE:HD12	2.31	0.45
1:C:101:ALA:O	1:C:105:VAL:HG23	2.16	0.45
1:C:189:PHE:HD1	1:C:611:MET:HG2	1.81	0.45
1:C:363:TRP:O	1:C:367:ILE:HG13	2.15	0.45
1:C:571:MET:HG3	1:D:404:MET:HE2	1.97	0.45
1:C:647:MET:HG3	1:D:552:ALA:HB1	1.98	0.45
1:D:194:GLY:HA3	1:D:235:GLY:CA	2.43	0.45
1:D:226:ILE:O	1:D:230:VAL:HG23	2.16	0.45
1:D:233:ASN:HA	1:D:237:VAL:CG2	2.46	0.45
1:D:361:SER:N	1:D:362:PRO:HD2	2.32	0.45
1:D:405:VAL:HG21	1:D:683:ALA:HB1	1.98	0.45
1:D:409:GLY:HA3	1:D:659:TRP:CE2	2.51	0.45
1:B:42:ILE:CD1	1:B:226:ILE:HG23	2.47	0.45
1:B:468:GLY:HA2	1:B:484:THR:HG21	1.99	0.45
1:B:707:LYS:O	1:B:711:VAL:HG23	2.16	0.45
1:C:278:VAL:HG21	1:C:353:LEU:HD23	1.98	0.45
1:C:448:LEU:O	1:C:451:VAL:HB	2.17	0.45
1:C:723:VAL:O	1:C:723:VAL:HG12	2.16	0.45
1:D:34:ARG:O	1:D:38:ILE:HG12	2.17	0.45
1:D:112:THR:HG21	1:D:117:PRO:CG	2.46	0.45
1:D:521:GLN:HG2	1:D:717:VAL:HG22	1.98	0.45
1:D:660:ASP:O	1:D:664:LYS:HG3	2.16	0.45
1:A:530:PRO:HB3	6:A:809:GQB:C08	2.47	0.45
1:B:717:VAL:HA	1:B:720:PHE:CZ	2.52	0.45
1:C:69:MET:HE2	1:C:74:TRP:HB2	1.99	0.45
1:C:248:PHE:CE1	1:C:252:ILE:HD11	2.51	0.45
1:D:102:ASN:HB2	1:D:466:ASN:HB3	1.99	0.45
1:D:376:ILE:HD11	1:D:424:LEU:HD11	1.98	0.45
1:D:390:PRO:HB2	1:D:412:LEU:HD11	1.99	0.45
1:A:370:ILE:O	1:A:374:ILE:HG13	2.17	0.45
1:A:500:GLY:O	1:A:503:ILE:HG22	2.16	0.45
1:B:6:LEU:O	1:B:6:LEU:HD23	2.17	0.45
1:B:252:ILE:HG23	1:B:290:PRO:HB2	1.99	0.45
1:D:84:ALA:CB	1:D:186:ILE:HG13	2.46	0.45
1:D:208:VAL:HG22	1:D:574:VAL:HG13	1.98	0.45
1:D:363:TRP:O	1:D:367:ILE:HG13	2.16	0.45
1:B:127:SER:HA	1:B:456:SER:HB2	1.98	0.45
1:B:167:ILE:HD11	1:B:719:ILE:CD1	2.31	0.45
1:C:202:ASP:HB2	8:C:902:HOH:O	2.15	0.45
1:C:223:PRO:CB	1:C:580:GLN:HE22	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:VAL:CG1	1:C:274:LEU:HB3	2.46	0.45
1:C:424:LEU:O	1:C:428:ILE:HG13	2.17	0.45
1:D:227:ALA:HA	1:D:600:ILE:CD1	2.46	0.45
1:D:301:SER:O	1:D:305:ILE:HG13	2.15	0.45
1:B:10:ILE:CG2	1:B:298:LEU:HD22	2.44	0.45
1:B:185:ILE:HG12	1:B:708:ILE:CD1	2.47	0.45
1:C:317:PRO:HG2	1:C:490:VAL:HG21	1.98	0.45
1:C:587:LEU:HD23	1:C:587:LEU:O	2.17	0.45
1:C:639:ILE:HD13	1:D:539:MET:HG3	1.99	0.45
1:D:224:ALA:CB	1:D:577:ILE:HD11	2.41	0.45
1:B:252:ILE:HG12	1:B:445:LEU:HD13	1.99	0.45
1:C:160:ILE:HG23	1:C:524:PRO:HB3	1.99	0.45
1:A:70:ILE:HG22	1:A:71:PHE:CD1	2.51	0.45
1:A:102:ASN:HB2	1:A:466:ASN:HB3	1.99	0.45
1:A:126:GLY:O	1:A:456:SER:HA	2.17	0.45
1:A:199:LYS:CD	1:A:696:ASP:HB2	2.41	0.45
1:A:301:SER:HB3	1:A:452:ALA:HB3	1.99	0.45
1:A:363:TRP:CE3	1:A:367:ILE:HD11	2.52	0.45
1:B:208:VAL:HG23	1:B:574:VAL:HG22	1.99	0.45
1:C:167:ILE:HG12	1:C:719:ILE:CG1	2.47	0.45
1:C:323:ILE:O	1:C:327:THR:HG23	2.17	0.45
1:C:444:ALA:HB2	1:C:508:PHE:HB2	1.94	0.45
1:C:651:LEU:HD23	1:C:651:LEU:C	2.37	0.45
1:D:129:MET:CE	1:D:241:GLY:HA3	2.47	0.45
1:D:149:GLY:CA	1:D:155:VAL:HG23	2.47	0.45
1:D:446:GLY:HA2	1:D:449:SER:HB3	1.97	0.45
1:D:685:VAL:O	1:D:689:THR:HG23	2.17	0.45
1:A:184:SER:OG	1:A:708:ILE:HG12	2.17	0.44
1:A:651:LEU:C	1:A:651:LEU:HD23	2.37	0.44
1:C:46:ALA:HB1	1:C:95:MET:SD	2.57	0.44
1:C:57:ILE:HG12	1:C:189:PHE:HB3	1.99	0.44
1:C:539:MET:CG	1:D:539:MET:HG2	2.40	0.44
1:A:17:PHE:HB3	1:A:131:LEU:HD13	1.99	0.44
1:A:32:THR:OG1	1:A:33:GLU:N	2.51	0.44
1:A:263:PHE:HB2	1:A:283:ILE:HG13	1.99	0.44
1:A:370:ILE:HG23	1:A:450:PHE:CE2	2.53	0.44
1:B:398:SER:HB2	1:B:684:LEU:HG	1.99	0.44
1:C:18:ALA:HB2	1:C:131:LEU:CB	2.47	0.44
1:C:355:PHE:CE1	1:C:362:PRO:HD3	2.52	0.44
1:C:448:LEU:CD1	1:C:505:SER:HB2	2.43	0.44
1:D:54:THR:O	1:D:57:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HA	1:A:596:TYR:HD1	1.82	0.44
1:A:249:VAL:O	1:A:253:VAL:HG23	2.16	0.44
1:A:569:ALA:HB2	1:A:606:ASN:ND2	2.31	0.44
1:A:573:MET:O	1:A:577:ILE:HG13	2.15	0.44
1:B:103:VAL:HG23	1:B:470:ILE:CD1	2.35	0.44
1:B:278:VAL:HG11	1:B:353:LEU:HD21	1.99	0.44
1:C:80:PHE:CE2	1:C:182:GLY:HA2	2.52	0.44
1:C:129:MET:HE1	1:C:241:GLY:HA3	1.99	0.44
1:C:149:GLY:O	1:C:155:VAL:HG23	2.16	0.44
1:C:216:PRO:HG2	1:C:219:ASP:HB2	1.97	0.44
1:C:227:ALA:HA	1:C:600:ILE:HD13	1.99	0.44
1:C:503:ILE:HD11	1:C:646:ALA:HA	1.98	0.44
1:C:535:LEU:HA	1:D:540:LEU:HD22	1.98	0.44
1:D:240:LEU:HD21	1:D:458:ASP:CG	2.37	0.44
1:D:337:ALA:HB2	1:D:363:TRP:CZ2	2.52	0.44
1:D:464:ALA:O	1:D:484:THR:HG23	2.17	0.44
1:A:57:ILE:CG1	1:A:189:PHE:HB3	2.47	0.44
1:A:141:LEU:HD21	1:A:252:ILE:CG2	2.48	0.44
1:A:199:LYS:HE2	1:A:199:LYS:CA	2.47	0.44
1:A:259:ALA:HB2	1:A:438:TYR:HE2	1.82	0.44
1:A:400:GLU:HG3	1:B:571:MET:CG	2.44	0.44
1:A:448:LEU:CD1	1:A:505:SER:HB2	2.46	0.44
1:B:619:ILE:CG1	1:B:708:ILE:HD11	2.48	0.44
1:C:6:LEU:HD23	1:C:6:LEU:O	2.18	0.44
1:C:265:ILE:HG22	1:C:531:PRO:HG3	1.99	0.44
1:D:53:GLU:OE2	1:D:193:GLY:HA3	2.17	0.44
1:D:344:LEU:HD22	1:D:347:LEU:HD11	1.99	0.44
1:A:410:LEU:O	1:A:414:MET:HG3	2.18	0.44
1:B:604:SER:O	1:B:608:LEU:HG	2.18	0.44
1:B:705:LEU:HA	1:B:708:ILE:HG22	1.99	0.44
1:C:47:ASP:OD1	1:C:95:MET:HE3	2.17	0.44
1:C:53:GLU:OE2	1:C:193:GLY:HA3	2.17	0.44
1:C:57:ILE:HG22	1:C:186:ILE:HD12	2.00	0.44
1:C:96:LYS:O	1:C:100:ARG:HG3	2.18	0.44
1:D:569:ALA:HB2	1:D:606:ASN:CB	2.47	0.44
1:A:62:ILE:O	1:A:66:ILE:HG12	2.17	0.44
1:A:95:MET:O	1:A:99:THR:HG23	2.18	0.44
1:A:101:ALA:O	1:A:105:VAL:HG23	2.17	0.44
1:A:139:LEU:HA	1:A:142:VAL:HG12	1.99	0.44
1:B:141:LEU:HD21	1:B:252:ILE:CG2	2.47	0.44
1:B:389:LYS:N	1:B:390:PRO:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:VAL:O	1:B:689:THR:HG23	2.17	0.44
1:C:115:ILE:HD12	1:C:115:ILE:N	2.32	0.44
1:C:221:ARG:O	1:C:587:LEU:HD21	2.17	0.44
1:C:613:TYR:N	1:C:614:PRO:HD2	2.32	0.44
1:D:196:VAL:HA	1:D:566:VAL:HG22	1.99	0.44
1:D:624:VAL:HG23	1:D:625:THR:N	2.33	0.44
1:A:23:ALA:HA	1:A:26:VAL:HG12	2.00	0.44
1:A:61:ALA:HB2	1:A:186:ILE:HD11	2.00	0.44
1:A:201:ALA:HB2	1:A:603:THR:HG21	2.00	0.44
1:A:227:ALA:HA	1:A:600:ILE:CD1	2.48	0.44
1:B:158:LEU:HD13	1:B:283:ILE:HG21	2.00	0.44
1:C:15:LEU:CD2	1:C:135:GLY:HA3	2.48	0.44
1:C:535:LEU:HB3	1:D:540:LEU:HD22	2.00	0.44
1:D:306:LEU:HA	1:D:309:ILE:HG12	2.00	0.44
1:A:208:VAL:HG21	1:A:574:VAL:HA	1.98	0.44
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.86	0.44
1:B:167:ILE:HD12	1:B:167:ILE:N	2.32	0.44
1:B:723:VAL:O	1:B:723:VAL:HG12	2.18	0.44
1:C:199:LYS:HE2	1:C:199:LYS:CA	2.47	0.44
1:C:386:TYR:CB	1:C:665:TYR:HB2	2.46	0.44
1:D:230:VAL:O	1:D:234:VAL:HG23	2.17	0.44
1:D:558:PHE:CD2	1:D:705:LEU:HD12	2.53	0.44
1:A:219:ASP:O	1:A:225:THR:HG21	2.18	0.44
1:A:227:ALA:HA	1:A:600:ILE:HD13	2.00	0.44
1:A:232:ASP:O	1:A:237:VAL:HG23	2.18	0.44
1:B:76:THR:OG1	1:B:174:MET:HG3	2.17	0.44
1:B:268:GLN:HG3	1:B:277:GLN:HG2	1.99	0.44
1:B:437:LEU:HD22	1:B:437:LEU:N	2.33	0.44
1:C:88:ALA:O	1:C:92:ILE:HG13	2.18	0.44
1:C:545:ILE:HG21	1:D:511:LEU:CD1	2.44	0.44
1:D:424:LEU:HD21	1:D:504:GLY:HA2	2.00	0.44
1:A:189:PHE:HE1	1:A:612:GLY:HA2	1.83	0.43
1:A:262:MET:O	1:A:266:TYR:HD2	2.01	0.43
1:A:395:GLY:O	1:A:398:SER:OG	2.22	0.43
1:B:21:ASN:CB	1:B:128:VAL:HG22	2.47	0.43
1:B:705:LEU:HD23	1:B:705:LEU:C	2.38	0.43
1:C:15:LEU:HD21	1:C:135:GLY:HA3	1.99	0.43
1:C:571:MET:HG3	1:D:404:MET:HE1	1.98	0.43
1:C:615:ALA:O	1:C:619:ILE:HG13	2.18	0.43
1:C:647:MET:HB3	1:D:556:TYR:CE1	2.53	0.43
1:C:693:PRO:O	1:C:697:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:618:ALA:HB1	1:D:708:ILE:CG2	2.48	0.43
1:A:344:LEU:O	1:A:359:ALA:HB2	2.18	0.43
1:A:511:LEU:HD12	1:B:545:ILE:HD13	2.00	0.43
1:B:23:ALA:HA	1:B:26:VAL:CG1	2.47	0.43
1:B:129:MET:HE1	1:B:241:GLY:H	1.83	0.43
1:B:500:GLY:O	1:B:503:ILE:HG22	2.19	0.43
1:C:399:ILE:HD13	1:C:680:PRO:CB	2.48	0.43
1:D:107:GLU:O	1:D:111:THR:HG23	2.18	0.43
1:A:266:TYR:CD1	1:A:531:PRO:HG2	2.54	0.43
1:A:580:GLN:HE22	1:A:595:ASP:HB3	1.82	0.43
1:A:624:VAL:HG23	1:A:625:THR:N	2.33	0.43
1:B:138:LEU:HD21	1:B:294:ALA:CB	2.46	0.43
1:B:170:VAL:HG13	1:B:171:PRO:HD2	2.00	0.43
1:C:481:ARG:HA	1:C:484:THR:OG1	2.18	0.43
1:C:558:PHE:CD2	1:C:705:LEU:HD12	2.54	0.43
1:D:188:MET:CB	1:D:704:ILE:HG21	2.46	0.43
1:D:359:ALA:O	1:D:362:PRO:HD2	2.18	0.43
1:B:34:ARG:O	1:B:38:ILE:HG13	2.18	0.43
1:C:80:PHE:CE2	1:C:185:ILE:HD12	2.51	0.43
1:C:500:GLY:O	1:C:503:ILE:HG22	2.17	0.43
1:C:624:VAL:HG23	1:C:625:THR:N	2.33	0.43
1:D:21:ASN:O	1:D:25:VAL:HG23	2.19	0.43
1:D:717:VAL:HA	1:D:720:PHE:CZ	2.54	0.43
1:B:350:LEU:HB3	1:B:355:PHE:HD2	1.83	0.43
1:B:448:LEU:O	1:B:451:VAL:HB	2.18	0.43
1:C:263:PHE:HB3	1:C:264:PRO:HD3	2.00	0.43
1:C:421:THR:CB	1:D:553:ALA:HB2	2.48	0.43
1:C:663:LYS:O	1:C:667:GLU:HG3	2.19	0.43
1:D:129:MET:HE1	1:D:241:GLY:N	2.34	0.43
1:D:325:LEU:HD23	1:D:453:THR:CG2	2.49	0.43
1:B:54:THR:HA	1:B:57:ILE:CG1	2.48	0.43
1:B:283:ILE:O	1:B:287:ILE:HG13	2.19	0.43
1:B:289:TYR:N	1:B:290:PRO:HD2	2.34	0.43
1:B:527:ILE:O	1:B:527:ILE:HG12	2.19	0.43
1:C:184:SER:HA	1:C:246:GLU:CG	2.43	0.43
1:C:306:LEU:HA	1:C:309:ILE:HG12	1.99	0.43
1:C:319:ARG:O	1:C:323:ILE:HG12	2.19	0.43
1:C:359:ALA:O	1:C:362:PRO:HD2	2.19	0.43
1:C:705:LEU:C	1:C:705:LEU:HD23	2.39	0.43
1:B:25:VAL:CG2	1:B:124:GLN:HB3	2.49	0.43
1:B:330:LEU:O	1:B:334:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:PHE:CZ	1:B:642:VAL:HG21	2.54	0.43
1:C:396:LYS:O	1:C:399:ILE:HG12	2.19	0.43
1:D:663:LYS:O	1:D:667:GLU:HG3	2.19	0.43
1:A:57:ILE:HG22	1:A:186:ILE:CD1	2.49	0.43
1:A:88:ALA:O	1:A:92:ILE:HG13	2.18	0.43
1:A:296:VAL:CG1	1:A:335:LEU:HB3	2.49	0.43
1:A:522:ILE:HD11	1:A:534:VAL:CG2	2.48	0.43
1:B:26:VAL:HG23	1:B:104:ARG:NH2	2.33	0.43
1:B:446:GLY:HA2	1:B:449:SER:HB3	1.99	0.43
1:C:185:ILE:HD13	1:C:619:ILE:CD1	2.49	0.43
1:C:597:ASN:ND2	1:C:597:ASN:O	2.51	0.43
1:C:628:LEU:O	1:C:629:LEU:HD23	2.19	0.43
1:C:638:LEU:HD11	1:C:713:SER:OG	2.19	0.43
1:D:289:TYR:N	1:D:290:PRO:HD2	2.34	0.43
1:D:325:LEU:HD23	1:D:453:THR:HG22	2.01	0.43
1:D:662:ALA:C	1:D:684:LEU:HD13	2.39	0.43
1:A:627:PHE:CD1	1:A:720:PHE:HB3	2.53	0.43
1:B:15:LEU:HD21	1:B:136:PHE:N	2.34	0.43
1:B:185:ILE:HD13	1:B:619:ILE:HD11	2.00	0.43
1:B:213:LEU:HB3	1:B:215:LEU:HD13	2.00	0.43
1:B:265:ILE:CG1	1:B:522:ILE:HD12	2.48	0.43
1:B:457:VAL:HG12	1:B:494:THR:HB	2.01	0.43
1:C:54:THR:HG22	1:C:58:PHE:HD2	1.83	0.43
1:C:386:TYR:HB2	1:C:665:TYR:HB2	2.01	0.43
1:D:477:ASP:OD1	1:D:478:PRO:HD2	2.19	0.43
1:D:527:ILE:O	1:D:527:ILE:HG12	2.18	0.43
1:D:559:SER:HB3	1:D:698:VAL:HG11	1.99	0.43
1:A:22:PHE:O	1:A:26:VAL:HG12	2.19	0.43
1:A:80:PHE:CE2	1:A:182:GLY:HA2	2.53	0.43
1:A:154:GLN:CG	1:A:171:PRO:HB2	2.49	0.43
1:A:363:TRP:O	1:A:367:ILE:HG13	2.18	0.43
1:B:261:TYR:O	1:B:265:ILE:HD13	2.19	0.43
1:C:417:VAL:CG2	1:C:651:LEU:HB2	2.49	0.43
1:C:425:VAL:HG21	1:D:550:LEU:HB2	2.00	0.43
1:D:167:ILE:CD1	1:D:719:ILE:HD11	2.49	0.43
1:D:223:PRO:HG2	1:D:577:ILE:HG12	2.00	0.43
1:D:584:ILE:HG22	1:D:587:LEU:HB2	2.01	0.43
1:A:6:LEU:HD23	1:A:6:LEU:O	2.19	0.42
1:B:141:LEU:CD2	1:B:252:ILE:HG21	2.49	0.42
1:B:213:LEU:HB2	1:B:215:LEU:HD13	2.00	0.42
1:B:370:ILE:O	1:B:374:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:PHE:HB3	1:B:419:PRO:CD	2.45	0.42
1:B:527:ILE:O	1:B:527:ILE:HG23	2.18	0.42
1:D:527:ILE:O	1:D:527:ILE:HG23	2.19	0.42
1:A:72:THR:HA	1:A:163:ASN:HD22	1.84	0.42
1:A:138:LEU:HD12	1:A:298:LEU:HD13	2.01	0.42
1:A:381:GLU:O	1:A:385:SER:HB3	2.19	0.42
1:B:199:LYS:HE2	1:B:199:LYS:CA	2.48	0.42
1:B:386:TYR:H	1:B:386:TYR:HD1	1.66	0.42
1:C:11:PRO:HD3	1:C:295:LEU:HD22	2.00	0.42
1:C:22:PHE:HD1	1:C:97:MET:SD	2.42	0.42
1:C:86:MET:HE2	1:C:136:PHE:O	2.18	0.42
1:C:129:MET:HE1	1:C:241:GLY:CA	2.49	0.42
1:C:149:GLY:CA	1:C:155:VAL:HG23	2.49	0.42
1:C:604:SER:O	1:C:608:LEU:HG	2.19	0.42
1:D:539:MET:CE	1:D:639:ILE:HG21	2.49	0.42
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.91	0.42
1:A:129:MET:CE	1:A:241:GLY:HA3	2.49	0.42
1:A:365:SER:O	1:A:368:ILE:HB	2.19	0.42
1:A:587:LEU:O	1:A:587:LEU:HD23	2.19	0.42
1:A:643:LEU:O	1:A:647:MET:HG2	2.18	0.42
1:B:119:LEU:HD13	1:B:317:PRO:CB	2.49	0.42
1:C:325:LEU:CD2	1:C:453:THR:HG22	2.46	0.42
1:D:389:LYS:N	1:D:390:PRO:HD2	2.35	0.42
1:D:424:LEU:CD2	1:D:507:ILE:HD12	2.49	0.42
1:A:213:LEU:CB	1:A:215:LEU:HD13	2.48	0.42
1:A:379:TRP:CE2	1:A:419:PRO:HB3	2.55	0.42
1:B:26:VAL:HG23	1:B:104:ARG:HH22	1.84	0.42
1:C:79:ALA:O	1:C:179:TYR:HA	2.18	0.42
1:C:117:PRO:O	1:C:121:VAL:HG12	2.19	0.42
1:C:527:ILE:O	1:C:527:ILE:HG12	2.20	0.42
1:C:539:MET:HG3	1:D:539:MET:CE	2.46	0.42
1:C:711:VAL:O	1:C:715:ILE:HG13	2.19	0.42
1:D:74:TRP:HH2	1:D:152:MET:CE	2.33	0.42
1:D:214:ASN:C	1:D:215:LEU:HD12	2.39	0.42
1:A:184:SER:HB2	1:A:708:ILE:HG13	2.01	0.42
1:A:320:GLU:OE1	1:A:320:GLU:HA	2.19	0.42
1:B:618:ALA:HB1	1:B:708:ILE:CG2	2.49	0.42
1:B:624:VAL:HG23	1:B:625:THR:N	2.35	0.42
1:C:386:TYR:HD2	1:C:665:TYR:CD2	2.36	0.42
1:C:630:GLY:H	1:C:724:HIS:CB	2.33	0.42
1:D:35:MET:HE1	1:D:476:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:HD1	1:A:234:VAL:HG11	1.80	0.42
1:A:117:PRO:O	1:A:121:VAL:HG12	2.19	0.42
1:B:165:LEU:HG	1:B:167:ILE:HD11	2.00	0.42
1:B:188:MET:CE	1:B:614:PRO:HB2	2.40	0.42
1:B:386:TYR:CB	1:B:665:TYR:HB2	2.49	0.42
1:B:444:ALA:HB2	1:B:508:PHE:HB2	2.00	0.42
1:B:481:ARG:HA	1:B:484:THR:OG1	2.19	0.42
1:C:188:MET:HE3	1:C:614:PRO:HB2	2.01	0.42
1:C:230:VAL:O	1:C:234:VAL:HG23	2.19	0.42
1:C:666:LEU:HD13	1:C:684:LEU:HD12	2.01	0.42
1:D:160:ILE:HG21	1:D:527:ILE:HD12	2.01	0.42
1:D:263:PHE:CE1	1:D:280:LYS:HG2	2.54	0.42
1:D:570:ALA:O	1:D:574:VAL:HG23	2.20	0.42
1:D:712:VAL:O	1:D:715:ILE:HG12	2.19	0.42
1:A:163:ASN:OD1	1:A:167:ILE:HB	2.20	0.42
1:A:227:ALA:HB2	1:A:600:ILE:HD13	2.02	0.42
1:A:414:MET:HG2	1:A:651:LEU:HD11	2.00	0.42
1:A:543:ARG:HH11	1:A:629:LEU:HB3	1.84	0.42
1:B:543:ARG:HH22	1:B:726:PHE:CB	2.32	0.42
1:C:23:ALA:HA	1:C:26:VAL:HG12	2.00	0.42
1:C:361:SER:N	1:C:362:PRO:HD2	2.34	0.42
1:C:401:GLY:O	1:C:405:VAL:HG23	2.19	0.42
1:C:550:LEU:O	1:C:554:ILE:HG13	2.19	0.42
1:D:8:PHE:CD2	1:D:146:LEU:HD21	2.55	0.42
1:D:86:MET:HE2	1:D:136:PHE:HB3	2.00	0.42
1:A:112:THR:HG21	1:A:117:PRO:HG2	2.01	0.42
1:A:232:ASP:O	1:A:236:ASP:HB2	2.20	0.42
1:A:248:PHE:CZ	1:A:294:ALA:HB1	2.54	0.42
1:A:361:SER:N	1:A:362:PRO:HD2	2.35	0.42
1:C:97:MET:HE2	1:C:125:GLY:HA2	2.02	0.42
1:D:86:MET:HE3	1:D:136:PHE:CD1	2.55	0.42
1:D:262:MET:SD	1:D:353:LEU:HD22	2.60	0.42
1:D:705:LEU:HA	1:D:708:ILE:HG22	2.01	0.42
1:D:707:LYS:O	1:D:711:VAL:HG23	2.20	0.42
1:B:31:GLY:CA	1:B:107:GLU:HG3	2.41	0.42
1:B:361:SER:N	1:B:362:PRO:HD2	2.35	0.42
1:B:386:TYR:HB2	1:B:665:TYR:HB2	2.02	0.42
1:C:141:LEU:CD2	1:C:252:ILE:HG21	2.50	0.42
1:C:555:THR:HG23	1:C:702:LEU:HD22	2.02	0.42
1:D:559:SER:HB3	1:D:698:VAL:CG1	2.49	0.42
1:A:253:VAL:O	1:A:257:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:O	1:A:262:MET:HG3	2.20	0.42
1:A:717:VAL:HG23	1:A:720:PHE:CE1	2.55	0.42
1:B:148:PHE:O	1:B:154:GLN:HB2	2.18	0.42
1:B:368:ILE:HG21	1:B:427:GLY:HA2	2.01	0.42
1:B:656:GLY:HA3	1:B:695:LYS:HB2	2.02	0.42
1:C:53:GLU:HG3	1:C:611:MET:CE	2.50	0.42
1:C:666:LEU:CD1	1:C:684:LEU:HD12	2.50	0.42
1:C:684:LEU:HD23	1:C:684:LEU:HA	1.89	0.42
1:D:95:MET:C	1:D:95:MET:HE2	2.41	0.42
1:D:201:ALA:HB2	1:D:603:THR:HG21	2.02	0.42
1:A:725:LEU:HD22	1:A:726:PHE:CZ	2.55	0.41
1:B:322:ASN:HD22	1:B:322:ASN:C	2.18	0.41
1:C:105:VAL:CG2	1:C:121:VAL:HG22	2.49	0.41
1:C:174:MET:SD	1:C:715:ILE:HG23	2.60	0.41
1:C:365:SER:O	1:C:368:ILE:HB	2.19	0.41
1:C:370:ILE:HG12	1:C:446:GLY:O	2.20	0.41
1:D:130:GLY:HA2	1:D:455:VAL:HB	2.02	0.41
1:D:417:VAL:HA	1:D:650:ILE:HG21	2.02	0.41
1:A:256:ILE:HG23	1:A:287:ILE:HG23	2.01	0.41
1:A:311:LYS:HG2	1:A:312:LYS:N	2.35	0.41
1:A:527:ILE:O	1:A:527:ILE:HG23	2.19	0.41
1:A:552:ALA:HB1	1:B:647:MET:HG3	2.02	0.41
1:B:230:VAL:O	1:B:234:VAL:HG23	2.19	0.41
1:C:90:ALA:HB1	1:C:133:VAL:HG22	2.01	0.41
1:C:282:THR:OG1	1:C:347:LEU:O	2.38	0.41
1:C:355:PHE:HB3	1:C:361:SER:HB2	2.02	0.41
1:C:643:LEU:CD1	1:D:643:LEU:HD12	2.48	0.41
1:D:563:ILE:HD11	1:D:694:LEU:HD23	2.01	0.41
1:A:226:ILE:HG13	1:A:473:MET:HE3	2.02	0.41
1:B:207:LEU:O	1:B:211:THR:HB	2.20	0.41
1:B:441:ALA:HB2	1:B:512:SER:OG	2.20	0.41
1:C:107:GLU:O	1:C:111:THR:HG23	2.20	0.41
1:C:630:GLY:H	1:C:724:HIS:HB3	1.83	0.41
1:D:573:MET:O	1:D:577:ILE:HG13	2.19	0.41
1:A:421:THR:CG2	1:B:553:ALA:HB2	2.45	0.41
1:B:9:LEU:O	1:B:13:VAL:HG23	2.20	0.41
1:B:54:THR:HG22	1:B:58:PHE:CD2	2.55	0.41
1:B:361:SER:HB3	1:B:435:ALA:HB2	2.01	0.41
1:C:686:ILE:O	1:C:690:VAL:HG23	2.20	0.41
1:D:188:MET:CA	1:D:704:ILE:HG21	2.50	0.41
1:D:205:ALA:HB2	1:D:224:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HD2	1:A:692:ASP:O	2.21	0.41
1:A:245:LEU:HD23	1:A:245:LEU:C	2.40	0.41
1:A:293:PHE:CZ	1:A:366:ALA:HB1	2.56	0.41
1:B:50:LEU:HD22	1:B:95:MET:SD	2.60	0.41
1:A:399:ILE:HD12	1:A:674:TYR:CD2	2.56	0.41
1:B:244:LEU:HD23	1:B:455:VAL:CG2	2.31	0.41
1:B:419:PRO:CD	1:B:420:PRO:HD2	2.50	0.41
1:B:663:LYS:O	1:B:667:GLU:HG3	2.21	0.41
1:C:168:ASN:H	1:C:718:SER:HB3	1.85	0.41
1:C:169:PHE:HB2	1:C:174:MET:CE	2.51	0.41
1:D:580:GLN:OE1	1:D:595:ASP:HB3	2.20	0.41
1:A:285:ALA:O	1:A:343:TYR:HE2	2.03	0.41
1:A:287:ILE:O	1:A:290:PRO:HD2	2.21	0.41
1:A:483:ILE:O	1:A:487:LEU:HG	2.21	0.41
1:A:557:TYR:CD1	1:B:415:LYS:HA	2.55	0.41
1:B:30:GLU:HG3	1:B:36:LYS:HE3	2.02	0.41
1:C:474:CYS:HB2	1:C:476:LEU:HD11	2.01	0.41
1:D:35:MET:HE2	1:D:476:LEU:HD11	2.02	0.41
1:D:39:SER:HA	1:D:42:ILE:CD1	2.48	0.41
1:D:95:MET:O	1:D:99:THR:HG23	2.21	0.41
1:D:350:LEU:HD12	1:D:350:LEU:N	2.36	0.41
1:A:289:TYR:N	1:A:290:PRO:HD2	2.36	0.41
1:A:564:SER:HB2	1:B:411:SER:OG	2.21	0.41
1:C:97:MET:HE3	1:C:125:GLY:CA	2.51	0.41
1:C:187:ALA:HA	1:C:242:ALA:HB1	2.03	0.41
1:D:205:ALA:HB2	1:D:224:ALA:HB3	2.01	0.41
1:D:386:TYR:HA	1:D:391:THR:HB	2.02	0.41
1:A:120:LYS:HE3	1:A:120:LYS:HB3	1.87	0.41
1:A:306:LEU:O	1:A:309:ILE:HG13	2.20	0.41
1:A:404:MET:SD	1:B:203:MET:HE2	2.61	0.41
1:A:406:ILE:HG21	1:B:690:VAL:HG11	2.02	0.41
1:A:641:THR:HG22	1:A:706:ILE:HG12	2.01	0.41
1:B:8:PHE:CD2	1:B:9:LEU:HD12	2.56	0.41
1:B:130:GLY:HA2	1:B:455:VAL:CG1	2.50	0.41
1:B:506:ALA:HB2	1:B:707:LYS:NZ	2.36	0.41
1:B:674:TYR:CD2	1:B:680:PRO:HG2	2.55	0.41
1:C:399:ILE:HD12	1:C:674:TYR:CE1	2.56	0.41
1:D:11:PRO:HD3	1:D:295:LEU:HD22	2.03	0.41
1:D:448:LEU:O	1:D:451:VAL:HB	2.20	0.41
1:D:587:LEU:O	1:D:587:LEU:HD23	2.21	0.41
1:D:651:LEU:C	1:D:651:LEU:HD23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TRP:HH2	1:A:152:MET:CE	2.34	0.41
1:B:149:GLY:HA2	1:B:155:VAL:HG23	2.02	0.41
1:B:170:VAL:HB	1:B:173:ALA:HB3	2.03	0.41
1:B:205:ALA:HB2	1:B:224:ALA:HB3	2.03	0.41
1:B:208:VAL:CG2	1:B:574:VAL:HG13	2.50	0.41
1:B:240:LEU:HD21	1:B:458:ASP:CG	2.41	0.41
1:B:627:PHE:HE1	1:B:719:ILE:CG2	2.32	0.41
1:B:698:VAL:O	1:B:702:LEU:HG	2.21	0.41
1:C:253:VAL:O	1:C:257:ILE:HG13	2.21	0.41
1:C:643:LEU:HD12	1:D:643:LEU:CD1	2.49	0.41
1:C:708:ILE:CG2	1:C:709:MET:N	2.84	0.41
1:D:337:ALA:HB2	1:D:363:TRP:CE2	2.56	0.41
1:D:376:ILE:HD11	1:D:424:LEU:CD1	2.50	0.41
1:A:356:ARG:HG3	1:A:357:PHE:CE1	2.56	0.40
1:A:471:SER:HA	1:A:476:LEU:CD1	2.47	0.40
1:A:690:VAL:HG11	1:B:406:ILE:HG21	2.03	0.40
1:B:25:VAL:CG1	1:B:97:MET:HE1	2.52	0.40
1:B:167:ILE:HA	1:B:718:SER:HB2	2.03	0.40
1:C:5:ALA:O	1:C:9:LEU:HD13	2.20	0.40
1:C:162:THR:HA	1:C:167:ILE:O	2.21	0.40
1:C:208:VAL:HG11	1:C:577:ILE:HG22	2.02	0.40
1:A:112:THR:CB	1:A:117:PRO:HG2	2.51	0.40
1:A:663:LYS:O	1:A:667:GLU:HG3	2.20	0.40
1:B:31:GLY:HA2	1:B:107:GLU:CG	2.40	0.40
1:C:25:VAL:HG21	1:C:97:MET:HE1	2.03	0.40
1:D:357:PHE:N	1:D:361:SER:OG	2.52	0.40
1:D:699:GLY:N	1:D:700:PRO:HD2	2.36	0.40
1:A:35:MET:HE1	1:A:110:ARG:HD3	2.03	0.40
1:A:185:ILE:HD13	1:A:619:ILE:CD1	2.49	0.40
1:A:717:VAL:HA	1:A:720:PHE:CE1	2.56	0.40
1:B:253:VAL:O	1:B:257:ILE:HG13	2.22	0.40
1:C:69:MET:HE3	1:C:74:TRP:HB2	2.03	0.40
1:C:262:MET:HE2	1:C:353:LEU:HD22	2.03	0.40
1:C:518:MET:HE2	1:C:534:VAL:O	2.20	0.40
1:D:84:ALA:HB1	1:D:186:ILE:HG13	2.03	0.40
1:D:131:LEU:HD22	1:D:302:MET:HG2	2.02	0.40
1:D:199:LYS:HD2	1:D:692:ASP:O	2.22	0.40
1:A:53:GLU:O	1:A:57:ILE:HG13	2.21	0.40
1:A:57:ILE:HD11	1:A:611:MET:CE	2.51	0.40
1:A:82:LEU:HD23	1:A:144:VAL:CG2	2.51	0.40
1:A:142:VAL:O	1:A:146:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASP:CG	1:A:220:PRO:HD2	2.42	0.40
1:B:210:LYS:HE2	1:B:217:GLU:HB2	2.02	0.40
1:B:356:ARG:HG3	1:B:357:PHE:CD1	2.56	0.40
1:B:522:ILE:HD11	1:B:534:VAL:CG2	2.51	0.40
1:B:543:ARG:HH22	1:B:726:PHE:C	2.25	0.40
1:C:157:ASN:OD1	1:C:158:LEU:N	2.52	0.40
1:C:633:PHE:O	1:C:637:VAL:HG23	2.22	0.40
1:D:54:THR:HG22	1:D:58:PHE:HD2	1.86	0.40
1:D:129:MET:HE1	1:D:241:GLY:HA3	2.03	0.40
1:D:382:TYR:HD1	1:D:388:TYR:CD2	2.39	0.40
1:D:442:ILE:HD13	1:D:442:ILE:HA	1.98	0.40
1:A:409:GLY:HA3	1:A:659:TRP:CZ2	2.57	0.40
1:B:192:VAL:O	1:B:196:VAL:HG23	2.21	0.40
1:B:307:TYR:CE1	1:B:311:LYS:HD3	2.57	0.40
1:B:402:THR:O	1:B:406:ILE:HG12	2.22	0.40
1:C:112:THR:CG2	1:C:117:PRO:HG2	2.52	0.40
1:C:125:GLY:HA3	1:C:463:ILE:CD1	2.52	0.40
1:C:246:GLU:OE2	1:C:707:LYS:HE2	2.22	0.40
1:C:584:ILE:HD13	1:C:584:ILE:HA	1.88	0.40
1:D:384:THR:HG21	1:D:493:THR:HA	2.04	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	723/735 (98%)	693 (96%)	30 (4%)	0	100	100
1	B	709/735 (96%)	679 (96%)	30 (4%)	0	100	100
1	C	723/735 (98%)	690 (95%)	33 (5%)	0	100	100
1	D	715/735 (97%)	685 (96%)	30 (4%)	0	100	100
All	All	2870/2940 (98%)	2747 (96%)	123 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	526/575 (92%)	523 (99%)	3 (1%)	86 94
1	B	519/575 (90%)	510 (98%)	9 (2%)	60 82
1	C	529/575 (92%)	525 (99%)	4 (1%)	81 92
1	D	518/575 (90%)	513 (99%)	5 (1%)	76 88
All	All	2092/2300 (91%)	2071 (99%)	21 (1%)	76 88

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	PHE
1	A	460	TYR
1	A	659	TRP
1	B	41	TYR
1	B	293	PHE
1	B	318	GLN
1	B	322	ASN
1	B	351	ASP
1	B	438	TYR
1	B	460	TYR
1	B	519	PHE
1	B	579	ARG
1	C	293	PHE
1	C	460	TYR
1	C	519	PHE
1	C	659	TRP
1	D	293	PHE
1	D	318	GLN
1	D	341	TYR
1	D	460	TYR
1	D	519	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	277	GLN
1	A	318	GLN
1	A	322	ASN
1	C	268	GLN
1	C	597	ASN
1	D	154	GLN
1	D	580	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 26 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
6	GQB	A	810	-	21,26,26	2.32	6 (28%)	27,37,37	2.90	11 (40%)
3	2PN	A	806	2,5	8,8,8	2.60	4 (50%)	8,13,13	1.40	0
7	D1D	C	807	-	6,8,8	2.60	4 (66%)	6,10,10	1.98	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GQB	A	809	-	21,26,26	2.29	6 (28%)	27,37,37	3.30	10 (37%)
6	GQB	C	808	-	21,26,26	2.31	5 (23%)	27,37,37	3.17	9 (33%)
3	2PN	C	806	2	8,8,8	2.60	4 (50%)	8,13,13	1.38	0
3	2PN	D	806	2,5	8,8,8	2.59	4 (50%)	8,13,13	1.43	0
3	2PN	B	806	2,5	8,8,8	2.61	4 (50%)	8,13,13	1.38	0

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
6	GQB	A	810	-	-	2/6/25/25	0/4/4/4
3	2PN	A	806	2,5	-	1/2/6/6	-
7	D1D	C	807	-	-	-	0/0/1/1
6	GQB	A	809	-	-	2/6/25/25	0/4/4/4
6	GQB	C	808	-	-	2/6/25/25	0/4/4/4
3	2PN	C	806	2	-	0/2/6/6	-
3	2PN	D	806	2,5	-	2/2/6/6	-
3	2PN	B	806	2,5	-	2/2/6/6	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	810	GQB	C02-N12	5.62	1.46	1.33
6	C	808	GQB	C02-N12	5.51	1.45	1.33
6	A	809	GQB	C02-N12	5.35	1.45	1.33
6	A	809	GQB	C13-C14	4.26	1.60	1.51
6	C	808	GQB	C21-N20	4.03	1.46	1.38
6	C	808	GQB	C13-C14	3.97	1.60	1.51
6	A	809	GQB	C21-N20	3.97	1.46	1.38
6	A	810	GQB	C21-N20	3.94	1.46	1.38
6	A	810	GQB	C13-C14	3.87	1.59	1.51
7	C	807	D1D	C3-C2	3.81	1.58	1.52
3	B	806	2PN	P1-O1	3.43	1.51	1.46
3	C	806	2PN	P1-O1	3.41	1.51	1.46
3	A	806	2PN	P1-O1	3.40	1.51	1.46
3	D	806	2PN	P1-O1	3.37	1.51	1.46
3	D	806	2PN	P2-O4	3.36	1.51	1.46
3	A	806	2PN	P2-O4	3.35	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	806	2PN	P2-O4	3.35	1.51	1.46
3	B	806	2PN	P2-O4	3.35	1.51	1.46
6	A	810	GQB	C13-N12	3.24	1.52	1.46
7	C	807	D1D	C4-C3	3.16	1.58	1.52
6	C	808	GQB	C13-N12	3.16	1.52	1.46
6	A	809	GQB	C18-N19	3.06	1.38	1.32
6	C	808	GQB	C18-N19	3.05	1.38	1.32
6	A	810	GQB	C18-N19	3.04	1.38	1.32
7	C	807	D1D	O2-C2	-3.01	1.37	1.43
6	A	809	GQB	C13-N12	2.89	1.51	1.46
3	B	806	2PN	P1-N1	2.88	1.70	1.63
3	C	806	2PN	P1-N1	2.84	1.70	1.63
3	A	806	2PN	P1-N1	2.84	1.70	1.63
3	B	806	2PN	P2-N1	2.83	1.70	1.63
3	A	806	2PN	P2-N1	2.82	1.70	1.63
3	D	806	2PN	P2-N1	2.81	1.70	1.63
3	C	806	2PN	P2-N1	2.81	1.70	1.63
3	D	806	2PN	P1-N1	2.79	1.70	1.63
7	C	807	D1D	O3-C3	-2.61	1.37	1.43
6	A	810	GQB	C09-C10	2.08	1.45	1.41
6	A	809	GQB	C09-C10	2.01	1.45	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	809	GQB	C03-C02-N12	11.77	132.07	115.59
6	C	808	GQB	C03-C02-N12	11.38	131.52	115.59
6	A	810	GQB	C03-C02-N12	8.83	127.94	115.59
6	C	808	GQB	N19-C18-N20	6.25	128.14	116.59
6	A	809	GQB	N19-C18-N20	6.23	128.12	116.59
6	A	810	GQB	N19-C18-N20	6.08	127.83	116.59
6	A	809	GQB	C16-C21-N20	4.91	117.93	112.13
6	A	810	GQB	C16-C21-N20	4.63	117.60	112.13
6	C	808	GQB	C16-C21-N20	4.59	117.55	112.13
6	A	809	GQB	O01-C02-N12	-4.27	114.09	122.61
6	C	808	GQB	O01-C02-N12	-4.25	114.14	122.61
6	A	810	GQB	C14-C13-N12	3.81	121.21	113.05
6	A	810	GQB	C03-N11-C10	3.63	112.03	104.45
6	A	809	GQB	C03-N11-C10	3.59	111.95	104.45
6	C	808	GQB	C03-N11-C10	3.52	111.79	104.45
6	A	810	GQB	O01-C02-N12	-3.42	115.78	122.61
6	A	810	GQB	C13-N12-C02	3.33	129.70	121.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	809	GQB	O01-C02-C03	-3.33	113.83	121.08
7	C	807	D1D	O3-C3-C2	-3.33	102.85	110.22
6	A	809	GQB	C22-C21-C16	-3.31	116.31	120.51
6	C	808	GQB	C22-C21-C16	-3.15	116.52	120.51
6	C	808	GQB	O01-C02-C03	-3.09	114.34	121.08
6	A	810	GQB	C22-C21-C16	-3.04	116.66	120.51
7	C	807	D1D	O2-C2-C1	-2.78	105.13	109.91
6	A	809	GQB	C13-C14-C15	2.71	126.50	120.64
6	A	810	GQB	C22-C21-N20	-2.52	125.74	130.87
6	A	809	GQB	C22-C21-N20	-2.51	125.76	130.87
6	A	809	GQB	C15-C16-C21	2.43	123.27	121.17
6	C	808	GQB	C22-C21-N20	-2.43	125.93	130.87
6	C	808	GQB	C15-C16-C21	2.37	123.22	121.17
6	A	810	GQB	C15-C16-C21	2.31	123.17	121.17
6	A	810	GQB	O01-C02-C03	-2.21	116.27	121.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	806	2PN	P2-N1-P1-O1
3	B	806	2PN	P1-N1-P2-O4
3	D	806	2PN	P2-N1-P1-O1
3	D	806	2PN	P1-N1-P2-O4
6	A	809	GQB	O01-C02-C03-C04
6	A	809	GQB	C14-C13-N12-C02
6	A	810	GQB	C14-C13-N12-C02
6	C	808	GQB	O01-C02-C03-C04
6	C	808	GQB	C14-C13-N12-C02
6	A	810	GQB	O01-C02-C03-C04
3	A	806	2PN	P2-N1-P1-O1

There are no ring outliers.

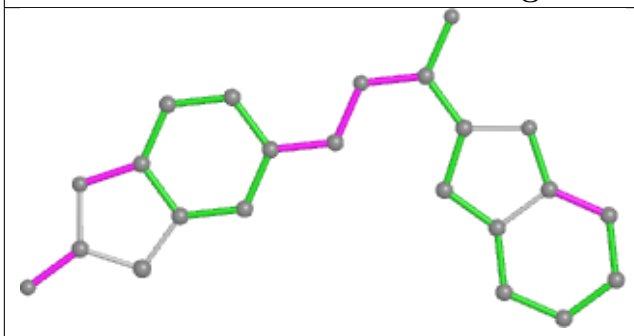
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	807	D1D	1	0
6	A	809	GQB	2	0

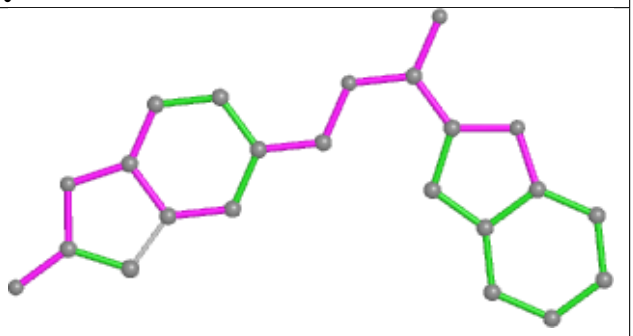
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

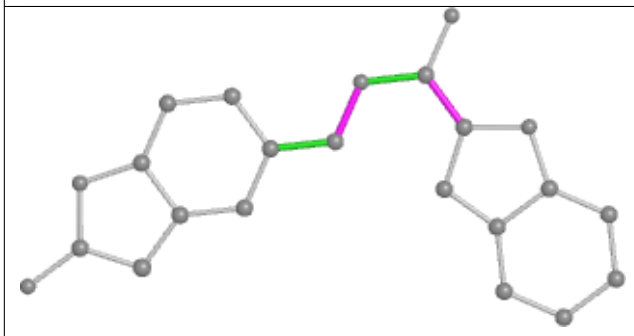
Ligand GQB A 810



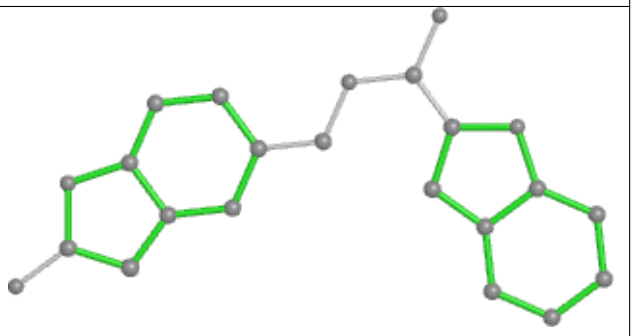
Bond lengths



Bond angles

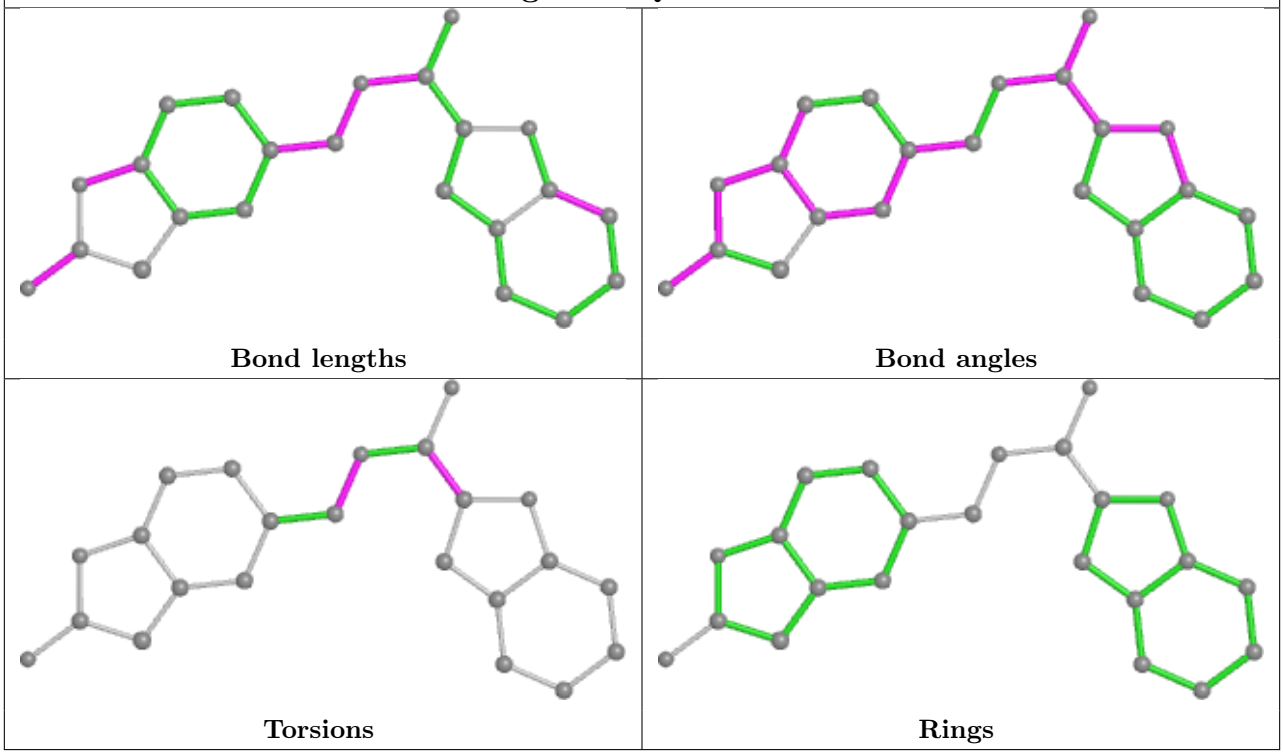


Torsions

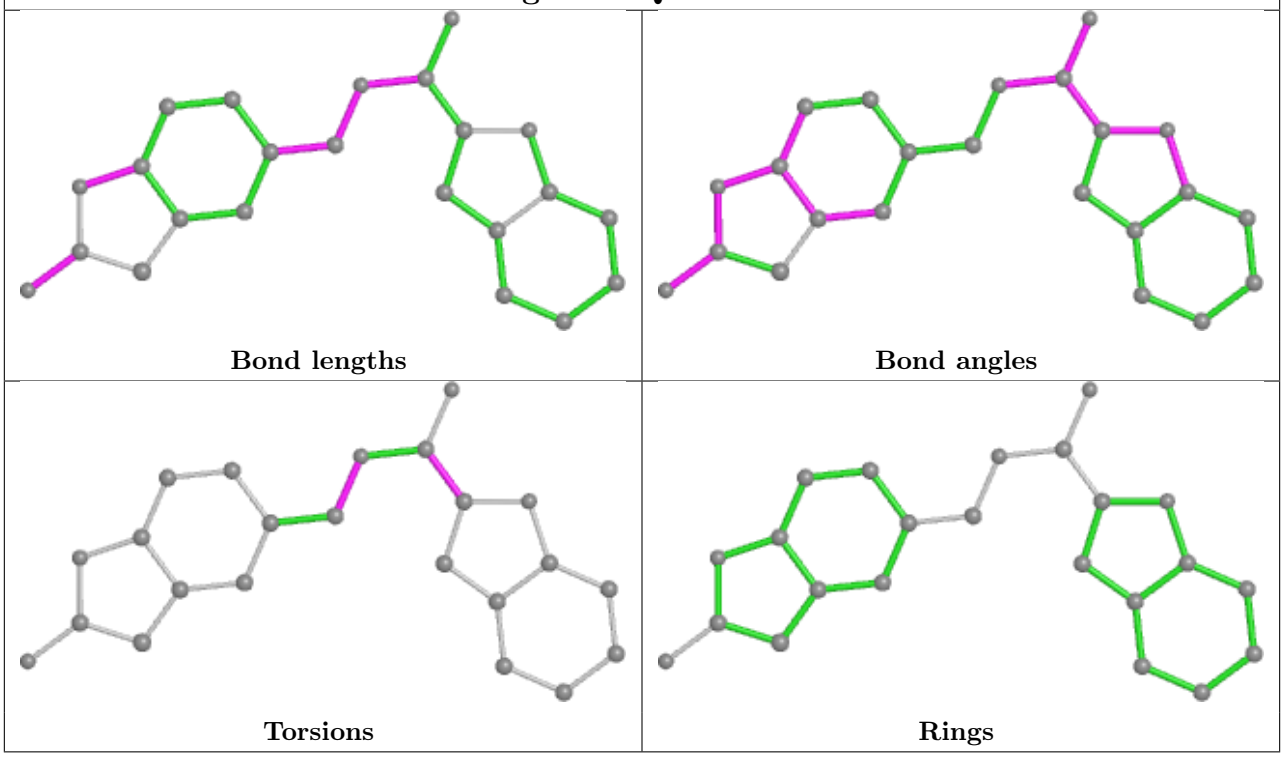


Rings

Ligand GQB A 809



Ligand GQB C 808



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

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	725/735 (98%)	0.29	43 (5%) 22 24	52, 79, 106, 148	0
1	B	715/735 (97%)	0.51	81 (11%) 5 7	56, 91, 127, 152	0
1	C	725/735 (98%)	0.24	50 (6%) 16 20	54, 81, 108, 135	0
1	D	719/735 (97%)	0.37	68 (9%) 8 10	53, 87, 111, 147	0
All	All	2884/2940 (98%)	0.35	242 (8%) 11 14	52, 85, 112, 152	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	592	ALA	7.6
1	D	587	LEU	6.8
1	B	359	ALA	6.7
1	B	474	CYS	5.7
1	B	350	LEU	5.6
1	B	587	LEU	5.6
1	B	588	LEU	5.6
1	D	585	PRO	5.4
1	B	594	PRO	5.4
1	A	272	GLU	5.4
1	D	588	LEU	5.3
1	D	599	CYS	5.3
1	C	674	TYR	5.2
1	B	599	CYS	5.2
1	C	675	GLY	4.9
1	D	589	GLU	4.9
1	D	584	ILE	4.9
1	B	592	ALA	4.8
1	D	586	GLY	4.8
1	B	595	ASP	4.7
1	D	6	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	580	GLN	4.6
1	B	597	ASN	4.6
1	A	527	ILE	4.6
1	B	278	VAL	4.4
1	B	584	ILE	4.3
1	B	9	LEU	4.3
1	B	355	PHE	4.3
1	A	722	HIS	4.3
1	B	8	PHE	4.2
1	B	277	GLN	4.2
1	A	670	ASN	4.2
1	C	268	GLN	4.1
1	A	523	SER	4.1
1	B	35	MET	4.0
1	B	107	GLU	4.0
1	B	34	ARG	3.9
1	A	674	TYR	3.9
1	B	351	ASP	3.9
1	B	352	VAL	3.9
1	C	274	LEU	3.8
1	B	475	GLU	3.8
1	A	723	VAL	3.8
1	C	477	ASP	3.8
1	A	526	ASP	3.7
1	B	585	PRO	3.7
1	B	354	GLY	3.7
1	C	30	GLU	3.7
1	B	110	ARG	3.6
1	B	268	GLN	3.6
1	B	267	VAL	3.6
1	C	670	ASN	3.5
1	B	353	LEU	3.5
1	D	726	PHE	3.5
1	B	36	LYS	3.5
1	D	315	ASP	3.5
1	B	109	ALA	3.4
1	B	358	GLY	3.4
1	A	270	ILE	3.4
1	B	530	PRO	3.4
1	B	589	GLU	3.4
1	D	578	ARG	3.3
1	C	267	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	30	GLU	3.3
1	B	360	ILE	3.3
1	B	586	GLY	3.3
1	D	590	GLY	3.3
1	B	526	ASP	3.2
1	D	118	ALA	3.2
1	D	522	ILE	3.2
1	D	301	SER	3.2
1	B	357	PHE	3.2
1	B	5	ALA	3.2
1	A	671	LEU	3.1
1	D	314	SER	3.1
1	D	596	TYR	3.1
1	D	594	PRO	3.1
1	D	7	PHE	3.1
1	A	666	LEU	3.1
1	D	577	ILE	3.1
1	D	8	PHE	3.1
1	A	3	VAL	3.1
1	C	527	ILE	3.1
1	B	111	THR	3.1
1	D	302	MET	3.1
1	B	7	PHE	3.1
1	C	157	ASN	3.1
1	D	576	GLU	3.0
1	C	672	GLU	3.0
1	D	313	PRO	3.0
1	C	25	VAL	3.0
1	C	533	LEU	3.0
1	D	222	ASN	3.0
1	D	117	PRO	3.0
1	C	531	PRO	3.0
1	D	531	PRO	3.0
1	C	29	PRO	3.0
1	D	349	GLY	3.0
1	B	522	ILE	3.0
1	C	160	ILE	2.9
1	B	523	SER	2.9
1	A	317	PRO	2.9
1	C	110	ARG	2.9
1	D	526	ASP	2.9
1	B	33	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	270	ILE	2.9
1	B	11	PRO	2.9
1	A	271	GLY	2.9
1	B	527	ILE	2.9
1	C	31	GLY	2.9
1	A	314	SER	2.9
1	A	590	GLY	2.9
1	C	400	GLU	2.8
1	C	474	CYS	2.8
1	C	386	TYR	2.8
1	B	473	MET	2.8
1	A	4	ALA	2.8
1	A	315	ASP	2.8
1	A	398	SER	2.8
1	D	247	SER	2.8
1	D	12	LEU	2.7
1	D	29	PRO	2.7
1	B	158	LEU	2.7
1	D	316	ASN	2.7
1	A	524	PRO	2.7
1	D	52	HIS	2.7
1	D	534	VAL	2.7
1	D	723	VAL	2.7
1	D	221	ARG	2.7
1	D	575	ASP	2.7
1	D	593	LYS	2.7
1	C	35	MET	2.7
1	B	12	LEU	2.7
1	B	596	TYR	2.6
1	D	348	GLN	2.6
1	A	613	TYR	2.6
1	C	401	GLY	2.6
1	C	269	LYS	2.6
1	C	671	LEU	2.6
1	C	505	SER	2.6
1	B	279	PRO	2.6
1	C	665	TYR	2.6
1	D	700	PRO	2.6
1	D	109	ALA	2.6
1	B	591	LYS	2.6
1	C	673	GLY	2.5
1	A	160	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	524	PRO	2.5
1	C	478	PRO	2.5
1	A	161	TYR	2.5
1	C	277	GLN	2.5
1	D	597	ASN	2.5
1	A	386	TYR	2.5
1	D	243	ASP	2.5
1	D	317	PRO	2.5
1	C	112	THR	2.5
1	C	667	GLU	2.5
1	B	525	SER	2.5
1	D	58	PHE	2.5
1	C	480	VAL	2.5
1	B	6	LEU	2.4
1	B	603	THR	2.4
1	B	117	PRO	2.4
1	B	725	LEU	2.4
1	D	17	PHE	2.4
1	C	381	GLU	2.4
1	A	23	ALA	2.4
1	B	41	TYR	2.4
1	C	524	PRO	2.4
1	D	527	ILE	2.4
1	A	669	GLY	2.4
1	C	399	ILE	2.4
1	D	268	GLN	2.4
1	B	243	ASP	2.4
1	C	678	SER	2.4
1	D	51	ALA	2.3
1	B	579	ARG	2.3
1	D	119	LEU	2.3
1	D	533	LEU	2.3
1	C	263	PHE	2.3
1	A	328	SER	2.3
1	B	3	VAL	2.3
1	B	593	LYS	2.3
1	C	530	PRO	2.3
1	B	103	VAL	2.3
1	D	672	GLU	2.3
1	C	111	THR	2.3
1	B	18	ALA	2.3
1	C	56	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	266	TYR	2.3
1	B	223	PRO	2.2
1	B	247	SER	2.2
1	C	276	HIS	2.2
1	A	579	ARG	2.2
1	B	4	ALA	2.2
1	D	53	GLU	2.2
1	D	580	GLN	2.2
1	C	216	PRO	2.2
1	A	127	SER	2.2
1	B	39	SER	2.2
1	A	307	TYR	2.2
1	C	109	ALA	2.2
1	A	313	PRO	2.2
1	D	277	GLN	2.2
1	B	310	VAL	2.2
1	D	570	ALA	2.1
1	B	726	PHE	2.1
1	B	703	ASP	2.1
1	D	581	ALA	2.1
1	A	324	SER	2.1
1	A	112	THR	2.1
1	D	310	VAL	2.1
1	C	669	GLY	2.1
1	D	208	VAL	2.1
1	D	267	VAL	2.1
1	A	321	LEU	2.1
1	A	665	TYR	2.1
1	A	522	ILE	2.1
1	A	213	LEU	2.1
1	A	589	GLU	2.1
1	B	476	LEU	2.1
1	B	309	ILE	2.1
1	D	583	GLU	2.1
1	D	160	ILE	2.1
1	D	699	GLY	2.1
1	C	155	VAL	2.1
1	D	574	VAL	2.1
1	B	365	SER	2.1
1	C	532	SER	2.1
1	A	243	ASP	2.1
1	D	703	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	676	LYS	2.0
1	B	344	LEU	2.0
1	C	279	PRO	2.0
1	A	581	ALA	2.0
1	A	676	LYS	2.0
1	A	719	ILE	2.0
1	B	467	ALA	2.0
1	D	4	ALA	2.0
1	B	362	PRO	2.0
1	A	326	TRP	2.0
1	B	308	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. 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	B-factors(Å^2)	Q<0.9
6	GQB	C	808	23/23	0.49	0.47	112,138,182,185	0
6	GQB	A	810	23/23	0.75	0.31	92,110,132,136	0
4	NA	D	807	1/1	0.84	1.02	74,74,74,74	0
6	GQB	A	809	23/23	0.85	0.27	68,104,127,139	0
5	K	D	808	1/1	0.87	0.34	92,92,92,92	0
2	MG	D	801	1/1	0.88	0.23	93,93,93,93	0
2	MG	A	801	1/1	0.89	0.15	68,68,68,68	0
2	MG	A	805	1/1	0.89	0.17	71,71,71,71	0
7	D1D	C	807	8/8	0.89	0.23	90,116,135,135	0
2	MG	B	804	1/1	0.91	0.61	85,85,85,85	0
5	K	A	808	1/1	0.93	0.28	110,110,110,110	0
2	MG	D	804	1/1	0.94	0.37	81,81,81,81	0

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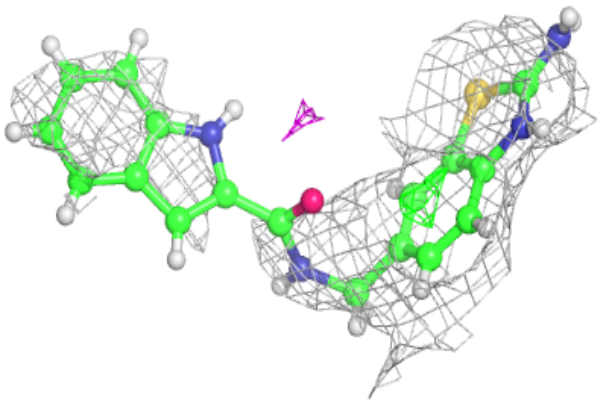
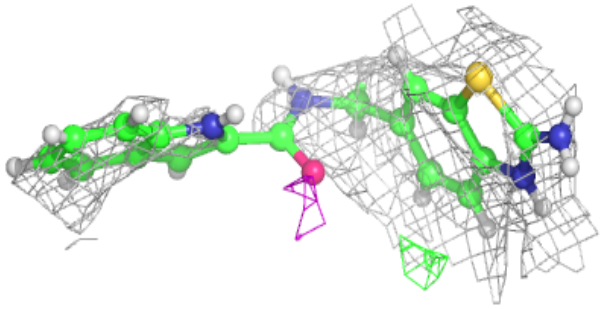
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	A	807	1/1	0.94	0.40	70,70,70,70	0
2	MG	D	803	1/1	0.94	0.47	97,97,97,97	0
2	MG	B	802	1/1	0.95	0.35	71,71,71,71	0
2	MG	B	803	1/1	0.95	0.33	78,78,78,78	0
2	MG	C	803	1/1	0.96	0.20	62,62,62,62	0
2	MG	A	802	1/1	0.96	0.25	78,78,78,78	0
2	MG	B	805	1/1	0.96	0.26	81,81,81,81	0
5	K	B	808	1/1	0.96	0.64	106,106,106,106	0
2	MG	C	802	1/1	0.96	0.29	72,72,72,72	0
2	MG	D	805	1/1	0.96	0.25	95,95,95,95	0
3	2PN	A	806	9/9	0.96	0.19	81,89,100,101	0
3	2PN	C	806	9/9	0.96	0.26	77,80,92,94	0
3	2PN	D	806	9/9	0.96	0.28	90,93,98,102	0
4	NA	B	807	1/1	0.97	0.62	68,68,68,68	0
2	MG	A	803	1/1	0.97	0.23	64,64,64,64	0
2	MG	C	805	1/1	0.97	0.10	73,73,73,73	0
2	MG	C	804	1/1	0.98	0.27	69,69,69,69	0
2	MG	D	802	1/1	0.98	0.28	87,87,87,87	0
2	MG	B	801	1/1	0.99	0.32	84,84,84,84	0
2	MG	C	801	1/1	0.99	0.18	65,65,65,65	0
2	MG	A	804	1/1	0.99	0.22	79,79,79,79	0
3	2PN	B	806	9/9	0.99	0.38	86,101,108,119	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GQB C 808:

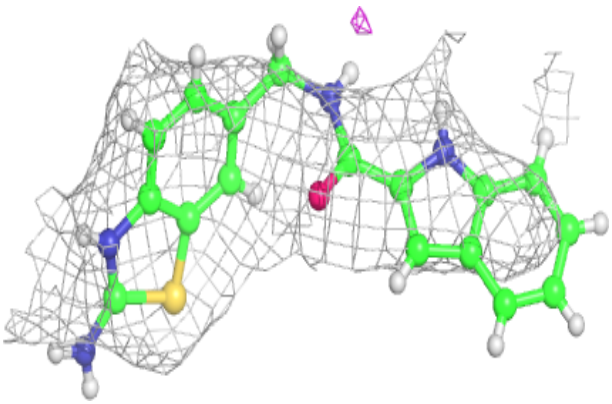
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

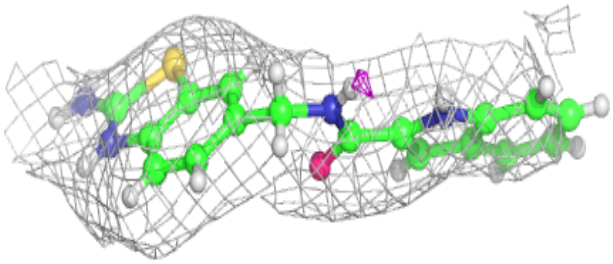


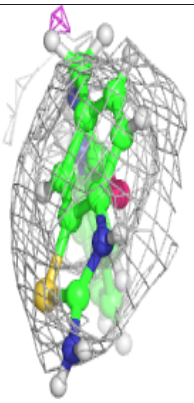


Electron density around GQB A 810:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

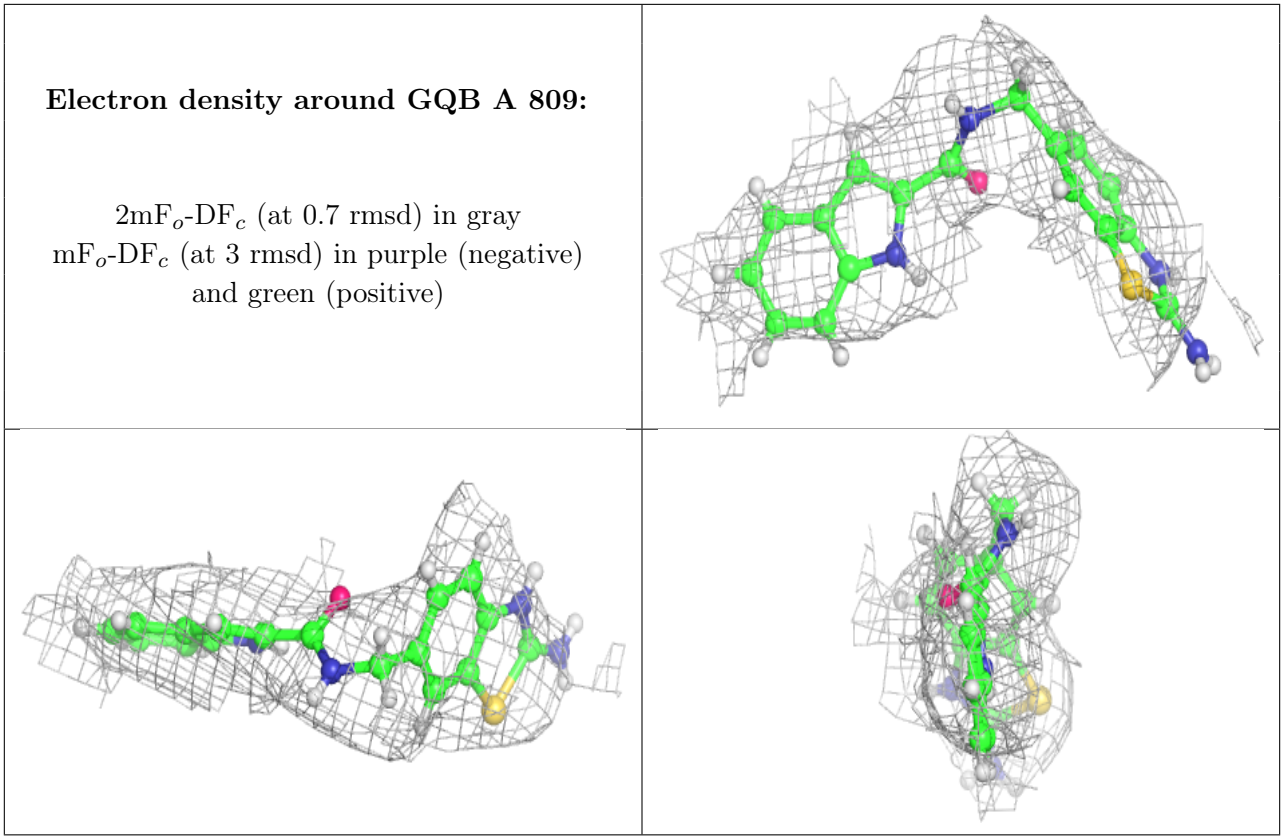






Electron density around GQB A 809:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.