Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 12:14 PM EST

PDB ID	:	4DOJ
Title	:	Crystal structure of BetP in outward-facing conformation
Authors	:	Perez, C.; Ziegler, C.
Deposited on	:	2012-02-09
Resolution	:	3.25 Å(reported)

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

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

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

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

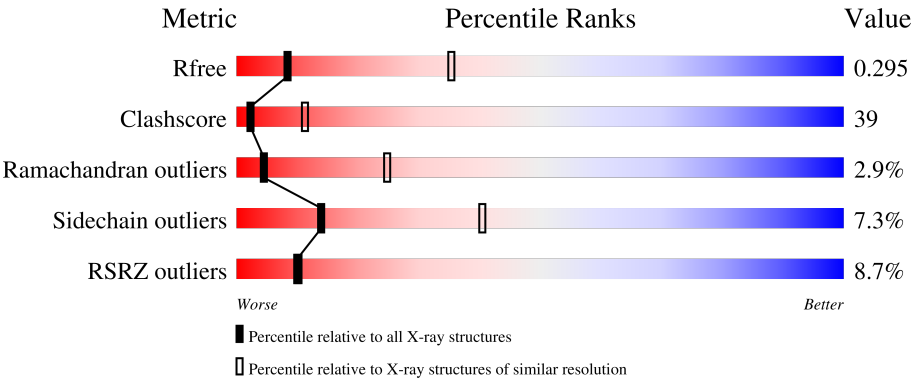
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	566	9% 39% 48% 6% 7%
1	B	566	11% 38% 42% 7% 11%
1	C	566	4% 38% 48% . 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11763 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycine betaine transporter BetP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			4017	2635	664	702	16			
1	B	501	Total	C	N	O	S	0	0	0
			3794	2502	607	669	16			
1	C	507	Total	C	N	O	S	0	0	0
			3860	2542	626	676	16			

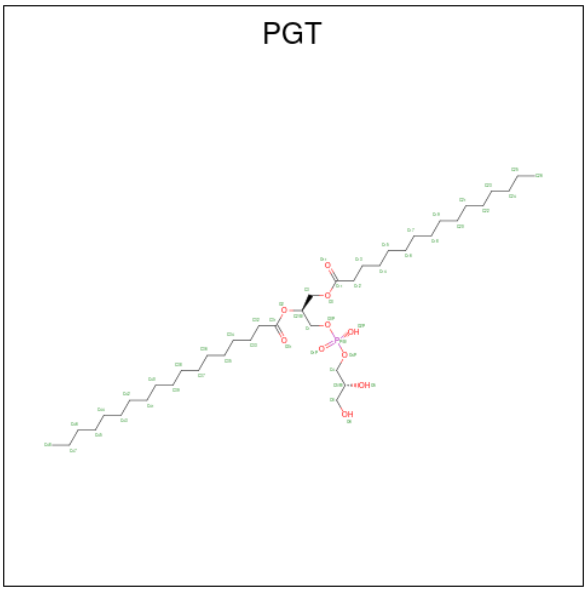
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLY	engineered mutation	UNP P54582
B	153	ASP	GLY	engineered mutation	UNP P54582
C	153	ASP	GLY	engineered mutation	UNP P54582

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

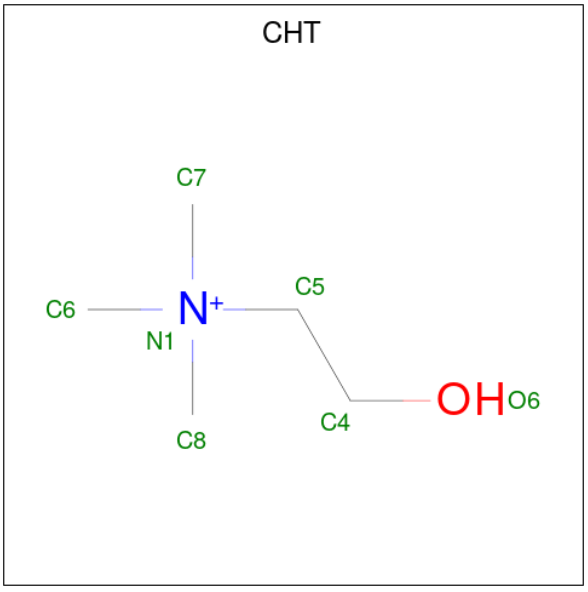
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	5	0
			51	40	10	1		

- Molecule 4 is CHOLINE ION (three-letter code: CHT) (formula: $C_5H_{14}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 5 is water.

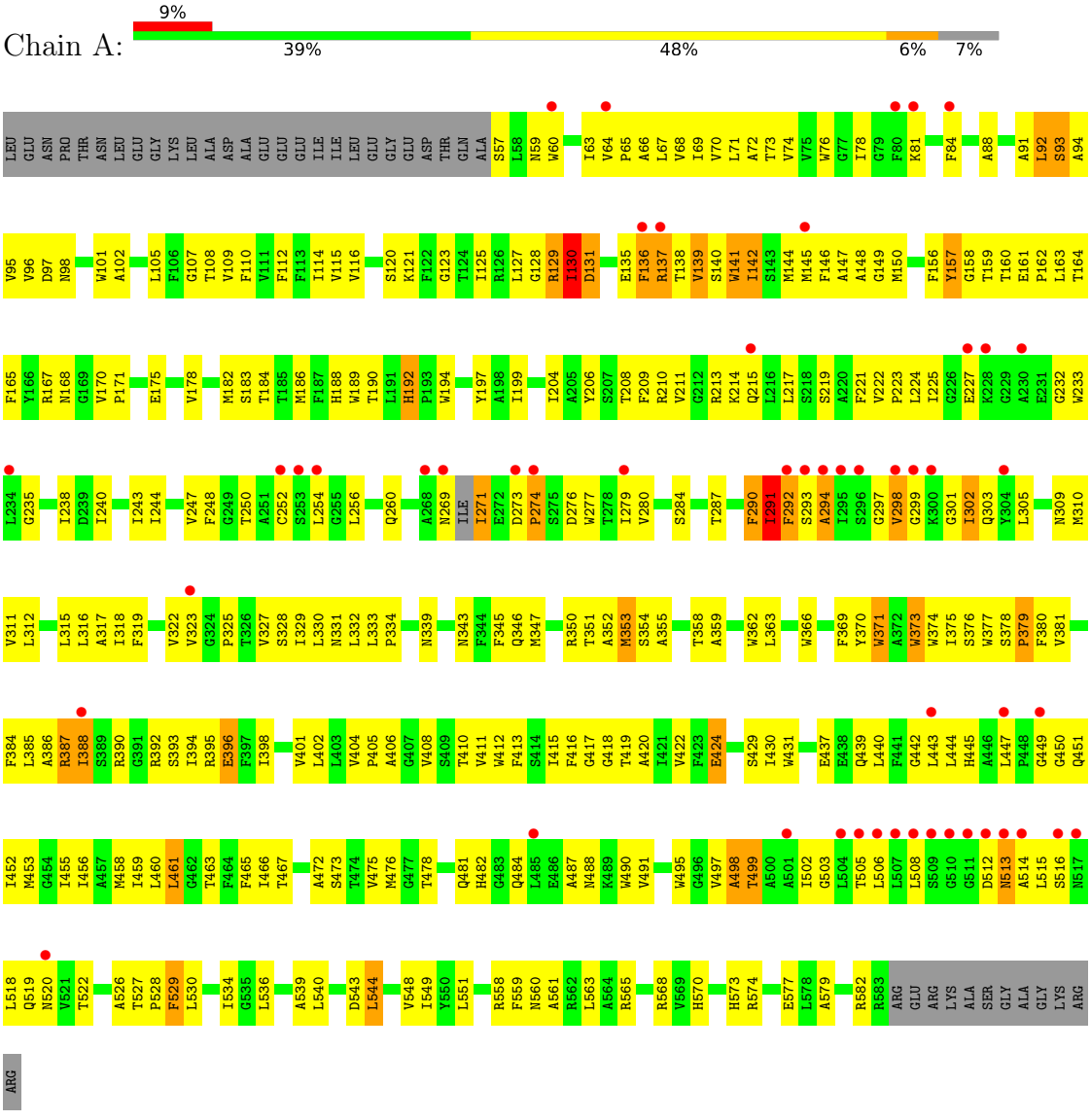
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	12	Total O 12 12	0	0
5	C	13	Total O 13 13	0	0

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.

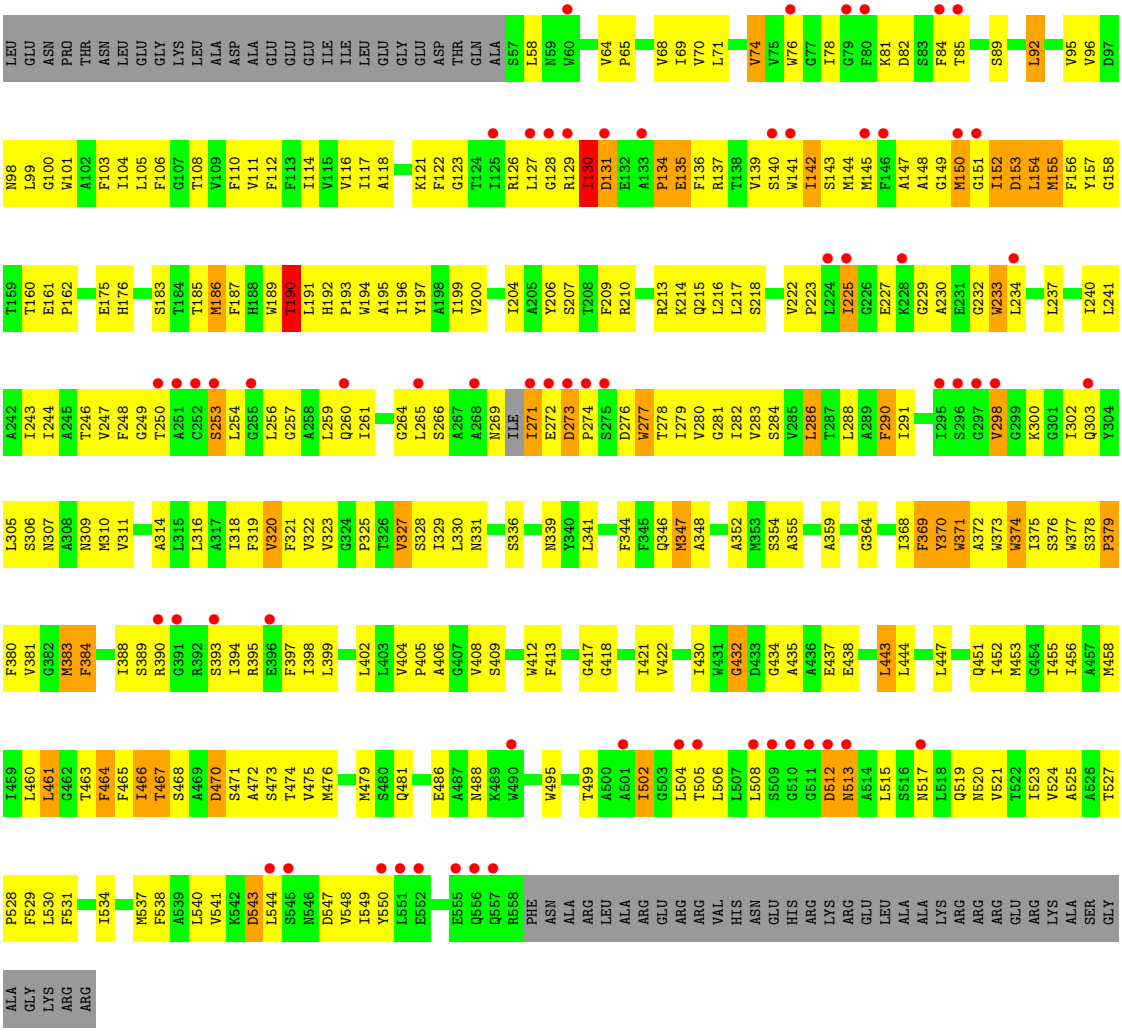
• Molecule 1: Glycine betaine transporter BetP

Chain A:



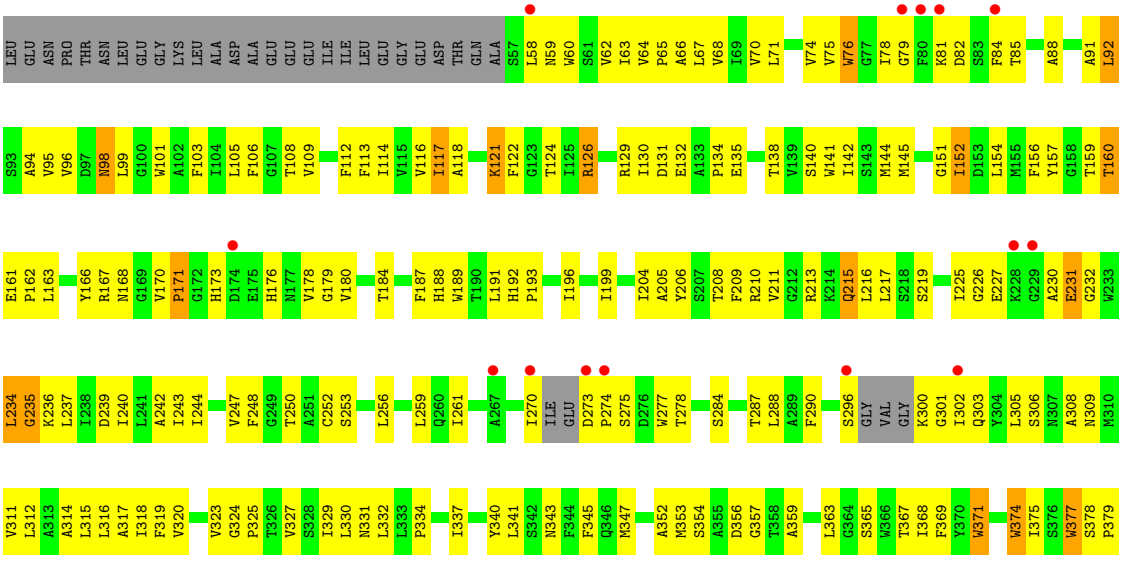
• Molecule 1: Glycine betaine transporter BetP

Chain B:



• Molecule 1: Glycine betaine transporter BetP

Chain C:




F380 V381 G382 M383 F384 L385 A386 R387 I388 S389 R390 G391 R395 E396 F397 I398 L399 G400 V401 V404 P405 T410 F413 S414 I415 F416 G417 G418 T419 A420 I421 V422 F423 E424 Q425 E428 S429 I430 W431 G432 D433 G434 A435 A436 E437 E438 Q439 L440 L443 L447 P448 G449 G450
Q451 I452 M453 G454 I455 I456 I459 L460 L461 G462 T463 F464 F465 I466 T467 S471 A472 S473 T474 V475 M476 M479 S480 Q481 H482 G483 Q484 L485 N488 V491 T492 A493 G496 I502 G503 L504 T505 L506 L507 L508 S509 N517 L518 Q519 N520 V521 T522 I523 V524 T527 P528
F529 L530 F531 V532 V533 I534 G535 L536 M537 F538 A539 L540 V541 K542 D543 L544 S545 N546 I549 Y550 L551 E552 Y553 R554 E555 Q556 Q557 R558 F559 N560 A561 R562 L563 A564 R565 E566 R567 R568 VAL HIS ASN GLU HIS ARG LYS ARG GLU LEU ALA ALA LYS ARG ARG ARG GLU ARG LYS ALA SER
GLY ALA GLY LYS ARG ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.44Å 129.32Å 184.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 3.25 46.28 – 3.21	Depositor EDS
% Data completeness (in resolution range)	86.0 (29.80-3.25) 82.7 (46.28-3.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	14.40 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.249 , 0.297 0.246 , 0.295	Depositor DCC
R_{free} test set	3848 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å^2)	79.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 110.8	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	0.88	EDS
Total number of atoms	11763	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: CHT, PGT, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.23	0/4119	0.40	0/5609
1	B	0.26	0/3892	0.41	0/5308
1	C	0.25	0/3958	0.43	0/5393
All	All	0.25	0/11969	0.41	0/16310

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	4017	0	4051	355	0
1	B	3794	0	3816	308	0
1	C	3860	0	3888	268	0
2	A	1	0	0	0	0
2	C	1	0	0	1	0
3	A	51	0	78	10	0
4	C	7	0	14	2	0
5	A	7	0	0	1	0
5	B	12	0	0	2	0
5	C	13	0	0	2	0
All	All	11763	0	11847	911	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 39.

All (911) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:H	1:A:298:VAL:CG2	1.52	1.21
1:A:506:LEU:O	1:A:506:LEU:HD23	1.37	1.18
1:C:226:GLY:HA2	1:C:227:GLU:HB3	1.29	1.07
1:A:292:PHE:H	1:A:293:SER:HB2	1.17	1.05
1:A:297:GLY:H	1:A:298:VAL:HG22	1.12	1.04
1:B:254:LEU:HD23	1:B:465:PHE:CE1	1.95	1.01
1:B:196:ILE:HD11	1:B:374:TRP:HB3	1.41	0.98
1:B:148:ALA:HB1	1:B:380:PHE:CZ	1.98	0.98
1:B:271:ILE:HG23	1:B:272:GLU:HA	1.42	0.98
1:B:254:LEU:HD23	1:B:465:PHE:CZ	1.98	0.98
1:B:261:ILE:HG13	1:B:282:ILE:HG21	1.45	0.98
1:A:370:TYR:HB3	1:A:374:TRP:HE1	1.24	0.97
1:A:297:GLY:N	1:A:298:VAL:CG2	2.30	0.95
1:C:95:VAL:HG21	1:C:527:THR:HG21	1.49	0.95
1:B:78:ILE:CG2	1:B:506:LEU:HD23	1.97	0.95
1:B:153:ASP:OD1	1:B:256:LEU:HG	1.70	0.91
1:B:453:MET:HE3	1:B:456:ILE:HD11	1.53	0.91
1:A:297:GLY:N	1:A:298:VAL:HG22	1.86	0.90
1:A:445:HIS:HA	1:A:450:GLY:HA3	1.53	0.90
1:A:252:CYS:SG	1:A:522:THR:HG21	2.12	0.89
1:A:302:ILE:HG22	1:A:303:GLN:H	1.38	0.87
1:B:154:LEU:HD12	1:B:154:LEU:O	1.73	0.87
1:A:292:PHE:N	1:A:293:SER:HB2	1.87	0.87
1:A:453:MET:O	1:A:456:ILE:HG12	1.76	0.85
1:A:297:GLY:H	1:A:298:VAL:HG23	1.40	0.85
1:B:152:ILE:HG12	1:B:464:PHE:HE1	1.41	0.85
1:A:141:TRP:CH2	1:A:392:ARG:HG2	2.11	0.85
1:C:78:ILE:HG23	1:C:505:THR:HG23	1.59	0.84
1:B:458:MET:HA	1:B:461:LEU:HD12	1.57	0.84
1:A:88:ALA:HB3	1:A:520:ASN:HD21	1.43	0.83
1:C:284:SER:HA	1:C:287:THR:HG22	1.58	0.83
1:C:237:LEU:O	1:C:240:ILE:HG22	1.77	0.83
1:A:312:LEU:HD13	1:A:460:LEU:HG	1.61	0.83
1:A:273:ASP:HB3	1:A:274:PRO:HD2	1.59	0.83
1:B:126:ARG:HD3	1:B:393:SER:HB3	1.61	0.81
1:C:375:ILE:HD13	1:C:530:LEU:HA	1.63	0.81
1:B:154:LEU:O	1:B:154:LEU:CD1	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:HA	1:B:393:SER:HA	1.63	0.80
1:C:167:ARG:HH22	1:C:431:TRP:HB2	1.45	0.80
1:B:271:ILE:HG12	1:B:273:ASP:H	1.47	0.80
1:A:312:LEU:HB3	1:A:460:LEU:CD2	2.12	0.80
1:C:160:THR:HG21	1:C:436:ALA:HB1	1.62	0.80
1:C:193:PRO:HB3	1:C:374:TRP:CD1	2.17	0.80
1:B:515:LEU:H	1:B:515:LEU:HD12	1.46	0.80
1:C:337:ILE:HD11	1:C:410:THR:HG21	1.61	0.79
1:A:387:ARG:O	1:A:388:ILE:HG12	1.82	0.79
1:B:154:LEU:HD12	1:B:154:LEU:C	2.01	0.78
1:A:490:TRP:HD1	1:A:491:VAL:HG13	1.47	0.78
1:A:392:ARG:HD2	1:A:396:GLU:HG3	1.63	0.78
1:B:298:VAL:HG12	1:B:298:VAL:O	1.82	0.78
1:B:141:TRP:CH2	1:B:389:SER:HB3	2.18	0.78
1:C:105:LEU:O	1:C:109:VAL:HG23	1.83	0.78
1:C:74:VAL:O	1:C:78:ILE:HG12	1.84	0.78
1:B:257:GLY:O	1:B:261:ILE:HG12	1.84	0.77
1:A:297:GLY:N	1:A:298:VAL:HG23	1.96	0.77
1:A:456:ILE:O	1:A:460:LEU:HB2	1.84	0.77
1:C:300:LYS:N	1:C:301:GLY:HA3	1.98	0.76
1:B:154:LEU:O	1:B:154:LEU:CG	2.30	0.76
1:A:505:THR:HA	1:A:508:LEU:HG	1.68	0.76
1:B:143:SER:HB2	1:B:306:SER:HB3	1.67	0.76
1:A:379:PRO:HG3	1:A:529:PHE:CZ	2.20	0.76
1:A:458:MET:HA	1:A:461:LEU:HD23	1.68	0.75
1:A:64:VAL:HB	1:A:65:PRO:HD3	1.68	0.75
1:C:163:LEU:HD22	1:C:420:ALA:HB1	1.68	0.75
5:B:607:HOH:O	1:C:354:SER:HB3	1.86	0.75
1:B:254:LEU:CD2	1:B:465:PHE:CZ	2.69	0.75
1:A:97:ASP:O	1:C:327:VAL:HG11	1.87	0.75
1:C:231:GLU:HA	1:C:235:GLY:HA3	1.67	0.75
1:B:290:PHE:HA	1:B:466:ILE:HD13	1.67	0.75
1:C:227:GLU:H	1:C:230:ALA:HB2	1.50	0.75
1:B:152:ILE:HG12	1:B:464:PHE:CE1	2.21	0.74
1:C:67:LEU:HA	1:C:70:VAL:HG12	1.68	0.74
1:B:418:GLY:O	1:B:422:VAL:HG23	1.87	0.74
1:C:559:PHE:HA	1:C:562:ARG:HG2	1.69	0.74
1:B:123:GLY:HA2	1:B:394:ILE:HD11	1.70	0.74
1:A:370:TYR:HB3	1:A:374:TRP:NE1	2.02	0.74
1:A:105:LEU:HB2	1:C:334:PRO:HB3	1.68	0.74
1:A:121:LYS:HG2	3:A:602:PGT:H11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:LEU:HB3	1:C:460:LEU:HD22	1.68	0.73
1:B:106:PHE:CD1	1:B:534:ILE:HD12	2.24	0.73
1:B:190:THR:HG22	1:B:406:ALA:HA	1.70	0.73
1:C:404:VAL:HB	1:C:405:PRO:HD3	1.71	0.73
1:B:161:GLU:HB3	1:B:162:PRO:HD3	1.71	0.73
1:A:506:LEU:HD23	1:A:506:LEU:C	2.09	0.73
1:C:506:LEU:HD23	1:C:518:LEU:HD12	1.69	0.73
1:A:209:PHE:CD2	1:A:390:ARG:HG2	2.24	0.72
1:B:153:ASP:C	1:B:155:MET:H	1.90	0.72
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.71	0.72
1:B:134:PRO:O	1:B:135:GLU:HB2	1.87	0.72
1:B:259:LEU:HD13	1:B:437:GLU:HG2	1.72	0.72
1:B:515:LEU:H	1:B:515:LEU:CD1	2.02	0.72
1:B:78:ILE:HG23	1:B:506:LEU:HD23	1.71	0.72
1:C:166:TYR:HA	5:C:701:HOH:O	1.89	0.72
1:B:271:ILE:CG2	1:B:272:GLU:HA	2.19	0.72
1:B:152:ILE:HG22	1:B:256:LEU:HD12	1.72	0.72
1:A:355:ALA:O	1:A:358:THR:HG22	1.90	0.71
1:B:261:ILE:HG21	1:B:282:ILE:HG12	1.71	0.71
1:B:150:MET:CE	1:B:154:LEU:CD2	2.69	0.71
1:C:211:VAL:HG11	1:C:213:ARG:CZ	2.20	0.71
1:A:68:VAL:HG13	1:A:69:ILE:HG13	1.71	0.71
1:B:101:TRP:HA	1:B:104:ILE:HD11	1.72	0.71
1:C:226:GLY:HA2	1:C:227:GLU:CB	2.05	0.71
1:A:305:LEU:HD22	1:A:467:THR:HG22	1.72	0.70
1:B:452:ILE:O	1:B:455:ILE:HG12	1.92	0.70
1:C:118:ALA:HB2	1:C:398:ILE:HD13	1.72	0.70
1:B:538:PHE:HA	1:B:541:VAL:HG12	1.73	0.70
1:A:260:GLN:HA	1:A:437:GLU:HG2	1.74	0.70
1:A:373:TRP:CD1	1:A:373:TRP:C	2.62	0.70
1:B:473:SER:HA	1:B:476:MET:SD	2.31	0.70
1:A:301:GLY:HA2	1:A:302:ILE:HB	1.74	0.69
1:C:343:ASN:O	1:C:347:MET:HG2	1.92	0.69
1:A:146:PHE:HZ	1:A:405:PRO:HA	1.56	0.69
1:B:150:MET:CE	1:B:154:LEU:HD22	2.22	0.69
1:C:523:ILE:O	1:C:527:THR:HG23	1.92	0.69
1:A:329:ILE:HG21	1:A:415:ILE:HG22	1.75	0.69
1:C:167:ARG:HG3	1:C:168:ASN:OD1	1.91	0.69
1:C:562:ARG:HA	1:C:565:ARG:HD2	1.75	0.69
1:B:256:LEU:HD22	1:B:259:LEU:HD21	1.73	0.69
1:A:506:LEU:O	1:A:506:LEU:CD2	2.30	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:TRP:O	1:B:190:THR:HG23	1.93	0.68
1:C:204:ILE:HD13	1:C:383:MET:HG2	1.74	0.68
1:B:110:PHE:HD1	1:B:196:ILE:HG22	1.57	0.68
1:B:141:TRP:HH2	1:B:389:SER:HB3	1.59	0.68
1:C:159:THR:HG21	1:C:443:LEU:HD22	1.75	0.68
1:C:452:ILE:O	1:C:456:ILE:HG13	1.94	0.68
1:B:225:ILE:HG21	1:B:230:ALA:HA	1.76	0.67
1:B:369:PHE:CD1	1:B:523:ILE:HD11	2.30	0.67
1:A:375:ILE:HG22	1:A:529:PHE:HB3	1.77	0.67
1:B:476:MET:HE2	1:B:495:TRP:HB3	1.77	0.67
1:B:515:LEU:HD12	1:B:515:LEU:N	2.10	0.67
1:C:140:SER:O	1:C:144:MET:HE2	1.94	0.67
1:C:243:ILE:O	1:C:247:VAL:HG23	1.94	0.67
1:A:183:SER:OG	1:A:339:ASN:HB3	1.94	0.67
1:A:316:LEU:HB3	1:A:456:ILE:HD11	1.77	0.67
1:B:341:LEU:HB3	1:C:345:PHE:CD2	2.29	0.67
1:B:384:PHE:CZ	1:B:471:SER:HB2	2.30	0.67
1:B:92:LEU:O	1:B:95:VAL:HG12	1.95	0.67
1:B:502:ILE:O	1:B:506:LEU:HG	1.94	0.67
1:A:384:PHE:O	1:A:387:ARG:HG2	1.95	0.66
1:B:154:LEU:O	1:B:154:LEU:HG	1.95	0.66
1:B:265:LEU:HD22	1:B:269:ASN:HD21	1.60	0.66
1:C:456:ILE:O	1:C:459:ILE:HG22	1.94	0.66
1:A:211:VAL:HG11	1:A:213:ARG:HE	1.60	0.66
1:C:485:LEU:H	1:C:485:LEU:HD12	1.60	0.66
1:A:312:LEU:HD22	1:A:460:LEU:HD11	1.77	0.66
1:A:150:MET:HE1	1:A:374:TRP:HZ3	1.60	0.66
1:C:122:PHE:CE1	1:C:544:LEU:HB3	2.30	0.66
1:C:354:SER:O	1:C:359:ALA:HB3	1.96	0.66
1:A:312:LEU:HB3	1:A:460:LEU:HD21	1.77	0.66
1:A:170:VAL:HG13	1:A:171:PRO:HD2	1.76	0.66
1:A:515:LEU:HD12	1:A:515:LEU:N	2.10	0.66
1:A:141:TRP:O	1:A:145:MET:HG2	1.95	0.66
1:B:152:ILE:CG1	1:B:464:PHE:HE1	2.09	0.66
1:B:300:LYS:HG3	1:B:303:GLN:HB2	1.77	0.66
1:B:453:MET:CE	1:B:456:ILE:HD11	2.25	0.66
1:C:473:SER:HA	1:C:476:MET:HE2	1.76	0.66
1:C:319:PHE:O	1:C:323:VAL:HG12	1.95	0.66
1:C:397:PHE:O	1:C:401:VAL:HG23	1.97	0.65
1:C:561:ALA:O	1:C:565:ARG:HG3	1.96	0.65
1:A:385:LEU:HD21	1:A:401:VAL:HG21	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:VAL:O	1:A:408:VAL:HG13	1.95	0.65
1:B:460:LEU:HA	1:B:463:THR:HG22	1.77	0.65
1:B:110:PHE:CD1	1:B:196:ILE:HG22	2.31	0.65
1:A:248:PHE:HB3	1:A:522:THR:HG22	1.77	0.65
1:A:252:CYS:HA	1:A:518:LEU:HD11	1.78	0.65
1:B:153:ASP:OD1	1:B:256:LEU:CG	2.45	0.65
1:C:261:ILE:HD11	1:C:461:LEU:HB2	1.79	0.65
1:B:254:LEU:HD23	1:B:465:PHE:HE1	1.58	0.65
1:C:296:SER:HG	1:C:300:LYS:N	1.95	0.65
1:C:319:PHE:CE2	1:C:453:MET:HG3	2.32	0.65
1:C:114:ILE:HD13	1:C:199:ILE:HD13	1.77	0.65
1:A:373:TRP:C	1:A:373:TRP:HD1	2.01	0.64
1:B:153:ASP:O	1:B:155:MET:N	2.29	0.64
1:B:323:VAL:HG23	1:B:447:LEU:HD22	1.78	0.64
1:C:81:LYS:HB3	1:C:84:PHE:CD2	2.32	0.64
1:A:463:THR:O	1:A:466:ILE:HG13	1.97	0.64
1:B:217:LEU:HD12	1:B:217:LEU:H	1.62	0.64
1:B:341:LEU:HD23	1:C:345:PHE:CZ	2.33	0.64
1:B:70:VAL:HG21	1:B:247:VAL:HG11	1.78	0.64
1:A:380:PHE:HA	1:A:475:VAL:HG11	1.79	0.64
1:C:163:LEU:HD11	1:C:424:GLU:HG3	1.78	0.64
1:A:316:LEU:HD12	1:A:317:ALA:N	2.13	0.63
1:B:470:ASP:O	1:B:474:THR:HG23	1.98	0.63
1:C:59:ASN:O	1:C:63:ILE:HG13	1.98	0.63
1:A:516:SER:HB3	1:A:519:GLN:HG2	1.80	0.63
1:B:460:LEU:O	1:B:463:THR:HG22	1.98	0.63
1:B:121:LYS:HZ1	1:B:550:TYR:HD1	1.47	0.63
1:B:150:MET:HE2	1:B:154:LEU:HD23	1.80	0.63
1:B:346:GLN:HG3	1:B:347:MET:N	2.14	0.63
1:B:378:SER:OG	1:B:379:PRO:HD3	1.99	0.63
1:B:149:GLY:C	1:B:150:MET:HG3	2.20	0.62
1:B:524:VAL:HA	1:B:527:THR:OG1	1.98	0.62
1:B:259:LEU:HD12	1:B:260:GLN:N	2.14	0.62
1:C:378:SER:N	1:C:379:PRO:HD2	2.14	0.62
1:A:206:TYR:CE1	1:A:210:ARG:HG2	2.34	0.62
1:A:449:GLY:O	1:A:452:ILE:HG12	1.99	0.62
1:A:373:TRP:HD1	1:A:373:TRP:O	1.81	0.62
1:A:404:VAL:HB	1:A:405:PRO:HD3	1.81	0.62
1:A:497:VAL:O	1:A:499:THR:HG22	2.00	0.62
1:B:152:ILE:CG2	1:B:256:LEU:HD12	2.29	0.62
1:C:273:ASP:HB2	1:C:274:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:PHE:HB3	1:C:522:THR:HG22	1.81	0.62
1:C:205:ALA:HB2	1:C:386:ALA:HA	1.82	0.61
1:B:144:MET:HA	1:B:147:ALA:HB3	1.82	0.61
1:C:108:THR:HA	1:C:192:HIS:CE1	2.36	0.61
1:C:208:THR:HG21	1:C:215:GLN:HG3	1.82	0.61
1:A:197:TYR:HH	1:A:374:TRP:HE3	1.48	0.61
1:A:243:ILE:HD12	1:A:244:ILE:N	2.15	0.61
1:A:463:THR:O	1:A:467:THR:HG23	1.99	0.61
1:B:517:ASN:O	1:B:521:VAL:HG23	2.01	0.61
1:A:114:ILE:HB	1:A:398:ILE:HD13	1.82	0.61
1:B:234:LEU:HD12	1:B:234:LEU:H	1.65	0.61
1:C:121:LYS:HD3	1:C:121:LYS:N	2.15	0.61
1:C:537:MET:O	1:C:541:VAL:HG23	2.00	0.61
1:C:539:ALA:O	1:C:543:ASP:HB2	2.00	0.61
1:A:69:ILE:HA	1:A:72:ALA:HB3	1.81	0.61
1:B:207:SER:O	1:B:213:ARG:HB2	2.01	0.61
1:C:126:ARG:HD3	1:C:132:GLU:O	2.00	0.61
1:A:146:PHE:CZ	1:A:405:PRO:HA	2.34	0.61
1:A:512:ASP:O	1:A:513:ASN:CB	2.48	0.61
1:C:549:ILE:HG13	2:C:602:CL:CL	2.37	0.61
1:A:149:GLY:HA2	1:A:381:VAL:HG12	1.83	0.61
1:A:354:SER:O	1:A:359:ALA:HB3	2.01	0.61
1:A:66:ALA:O	1:A:70:VAL:HG23	2.01	0.60
1:A:291:ILE:HB	1:A:294:ALA:HB2	1.83	0.60
1:C:71:LEU:HA	1:C:74:VAL:HG22	1.82	0.60
1:C:300:LYS:HD2	1:C:302:ILE:HG22	1.83	0.60
1:A:144:MET:HB3	1:A:384:PHE:CE2	2.36	0.60
1:A:316:LEU:O	1:A:319:PHE:HB3	2.01	0.60
1:A:138:THR:O	1:A:140:SER:N	2.33	0.60
1:B:260:GLN:CD	1:B:461:LEU:HD13	2.22	0.60
1:B:192:HIS:HB2	1:B:193:PRO:HD3	1.83	0.60
1:B:216:LEU:HD23	1:B:218:SER:H	1.67	0.60
1:B:404:VAL:HB	1:B:405:PRO:HD3	1.83	0.60
1:A:92:LEU:HD12	1:A:93:SER:N	2.17	0.60
1:A:165:PHE:CE1	1:A:362:TRP:HZ2	2.20	0.60
1:A:456:ILE:HB	1:A:460:LEU:HD22	1.82	0.60
1:C:64:VAL:CG1	1:C:65:PRO:HD3	2.32	0.60
1:C:230:ALA:O	1:C:231:GLU:HB3	2.01	0.60
1:C:381:VAL:HG12	1:C:385:LEU:HD12	1.84	0.59
1:B:78:ILE:HG22	1:B:506:LEU:HA	1.83	0.59
1:C:302:ILE:O	1:C:306:SER:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ILE:HG13	1:A:416:PHE:CD2	2.37	0.59
1:B:376:SER:O	1:B:379:PRO:HD2	2.03	0.59
1:A:142:ILE:HD13	1:A:142:ILE:H	1.66	0.59
1:B:463:THR:C	1:B:465:PHE:H	2.06	0.59
1:B:157:TYR:HA	1:B:160:THR:HG22	1.82	0.59
1:A:81:LYS:CB	1:A:84:PHE:HB2	2.33	0.59
1:C:122:PHE:CD1	1:C:544:LEU:HB3	2.37	0.59
1:A:527:THR:N	1:A:528:PRO:HD2	2.18	0.59
1:C:226:GLY:CA	1:C:227:GLU:HB3	2.20	0.59
1:A:141:TRP:HH2	1:A:392:ARG:HG2	1.64	0.59
1:A:158:GLY:HA2	1:A:413:PHE:HE1	1.68	0.59
1:A:330:LEU:HG	1:B:101:TRP:CD2	2.38	0.59
1:C:430:ILE:HD13	1:C:443:LEU:HB2	1.84	0.59
1:A:490:TRP:CD1	1:A:491:VAL:HG13	2.35	0.58
1:A:526:ALA:HB1	1:A:529:PHE:HB2	1.85	0.58
1:B:271:ILE:HG12	1:B:273:ASP:N	2.17	0.58
1:B:307:ASN:O	1:B:311:VAL:HG23	2.04	0.58
1:A:311:VAL:O	1:A:315:LEU:HB2	2.04	0.58
1:C:92:LEU:O	1:C:95:VAL:HG12	2.04	0.58
1:C:121:LYS:HD3	1:C:121:LYS:H	1.66	0.58
1:C:170:VAL:CG1	1:C:171:PRO:HD2	2.33	0.58
1:B:92:LEU:HD13	1:B:523:ILE:HG21	1.85	0.58
1:A:115:VAL:HG11	3:A:602:PGT:H402	1.85	0.58
1:A:123:GLY:O	1:A:395:ARG:HB2	2.02	0.58
1:A:302:ILE:HG22	1:A:303:GLN:N	2.15	0.58
1:A:579:ALA:O	1:A:582:ARG:HG2	2.03	0.58
1:C:252:CYS:SG	1:C:522:THR:HG21	2.43	0.58
1:B:472:ALA:O	1:B:476:MET:HG3	2.03	0.58
1:C:121:LYS:H	1:C:121:LYS:CD	2.15	0.58
1:A:71:LEU:HA	1:A:74:VAL:HB	1.85	0.58
1:B:331:ASN:OD1	1:C:101:TRP:HB3	2.03	0.58
1:A:161:GLU:HA	1:A:164:THR:HG22	1.86	0.58
1:A:478:THR:HG23	1:A:484:GLN:O	2.04	0.58
1:B:254:LEU:CD2	1:B:465:PHE:HZ	2.17	0.58
1:B:379:PRO:HG3	1:B:529:PHE:CZ	2.39	0.58
1:A:73:THR:HA	1:A:76:TRP:HB3	1.86	0.58
1:A:424:GLU:OE1	1:A:429:SER:HA	2.04	0.58
1:C:380:PHE:HE1	1:C:471:SER:HB2	1.68	0.57
1:C:226:GLY:O	1:C:230:ALA:HA	2.04	0.57
1:A:276:ASP:CG	1:A:277:TRP:H	2.08	0.57
1:B:144:MET:SD	1:B:388:ILE:HD12	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:HG3	1:A:529:PHE:CE2	2.39	0.57
1:C:290:PHE:CZ	1:C:493:ALA:HA	2.39	0.57
1:A:530:LEU:O	1:A:534:ILE:HG12	2.04	0.57
1:A:209:PHE:CE2	1:A:390:ARG:HG2	2.40	0.57
1:C:58:LEU:HA	1:C:481:GLN:HB3	1.86	0.57
1:B:148:ALA:HB1	1:B:380:PHE:HZ	1.60	0.57
1:A:128:GLY:HA2	1:A:209:PHE:O	2.05	0.57
1:A:112:PHE:CD1	3:A:602:PGT:H422	2.40	0.57
1:A:378:SER:HA	1:A:381:VAL:HG22	1.85	0.57
1:A:442:GLY:HA2	1:A:445:HIS:CD2	2.39	0.57
1:B:223:PRO:HG2	1:B:543:ASP:HB2	1.86	0.57
1:B:237:LEU:O	1:B:241:LEU:HG	2.04	0.57
1:C:92:LEU:HD13	1:C:520:ASN:HA	1.87	0.57
1:C:369:PHE:HA	1:C:523:ILE:HD11	1.86	0.57
1:B:215:GLN:HE21	1:B:383:MET:HG3	1.69	0.57
1:B:266:SER:OG	1:B:271:ILE:HG13	2.05	0.57
1:C:167:ARG:NH2	1:C:431:TRP:HB2	2.17	0.57
1:A:387:ARG:NH1	1:A:387:ARG:HB3	2.19	0.56
1:B:499:THR:O	1:B:502:ILE:HG12	2.05	0.56
1:C:227:GLU:H	1:C:230:ALA:CB	2.18	0.56
1:C:309:ASN:HB3	1:C:464:PHE:CE1	2.40	0.56
1:A:92:LEU:C	1:A:94:ALA:H	2.08	0.56
1:A:197:TYR:CE1	1:A:381:VAL:HG21	2.40	0.56
1:A:350:ARG:HG2	1:A:363:LEU:HD21	1.85	0.56
1:A:353:MET:HG2	1:C:332:LEU:HD21	1.87	0.56
1:B:190:THR:O	1:B:193:PRO:HD2	2.05	0.56
1:B:233:TRP:HD1	1:B:233:TRP:H	1.54	0.56
1:B:154:LEU:HD11	1:B:412:TRP:CD1	2.40	0.56
1:B:276:ASP:C	1:B:278:THR:H	2.09	0.56
1:C:248:PHE:CD1	1:C:502:ILE:HD12	2.41	0.56
1:B:150:MET:HE3	1:B:154:LEU:HD22	1.87	0.56
1:C:209:PHE:CE1	1:C:390:ARG:HB2	2.41	0.56
1:A:136:PHE:O	1:A:137:ARG:HB3	2.05	0.56
1:A:488:ASN:HB3	1:A:490:TRP:NE1	2.20	0.56
1:A:565:ARG:HD2	5:A:707:HOH:O	2.05	0.56
1:B:195:ALA:O	1:B:199:ILE:HD13	2.06	0.56
1:B:417:GLY:O	1:B:421:ILE:HG12	2.05	0.56
1:C:64:VAL:HG13	1:C:65:PRO:HD3	1.86	0.56
1:A:415:ILE:HG13	1:A:416:PHE:HD2	1.70	0.56
1:B:476:MET:HE2	1:B:495:TRP:HE3	1.69	0.56
1:C:157:TYR:O	1:C:161:GLU:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:HB3	1:A:384:PHE:HE2	1.70	0.56
1:A:252:CYS:SG	1:A:522:THR:CG2	2.89	0.56
1:A:334:PRO:HB3	1:B:105:LEU:HD13	1.88	0.56
1:C:167:ARG:HH22	1:C:431:TRP:CB	2.16	0.56
1:B:223:PRO:CG	1:B:543:ASP:HB2	2.36	0.55
1:A:392:ARG:CD	1:A:396:GLU:HG3	2.35	0.55
1:B:464:PHE:O	1:B:468:SER:OG	2.24	0.55
1:A:558:ARG:O	1:A:561:ALA:HB3	2.05	0.55
1:B:118:ALA:HB2	1:B:398:ILE:HD12	1.88	0.55
1:B:527:THR:HB	1:B:528:PRO:HD3	1.87	0.55
1:C:481:GLN:OE1	1:C:484:GLN:HB2	2.06	0.55
1:A:331:ASN:ND2	1:B:352:ALA:HB3	2.22	0.55
1:A:163:LEU:HD11	1:A:424:GLU:OE2	2.06	0.55
1:C:381:VAL:HG12	1:C:385:LEU:CD1	2.36	0.55
1:C:475:VAL:O	1:C:479:MET:HG2	2.05	0.55
1:B:254:LEU:HD23	1:B:465:PHE:HZ	1.65	0.55
1:B:504:LEU:HD12	1:B:505:THR:HG23	1.89	0.55
1:A:81:LYS:HB2	1:A:84:PHE:HB2	1.89	0.55
1:A:297:GLY:CA	1:A:298:VAL:CG2	2.85	0.55
1:B:521:VAL:O	1:B:525:ALA:HB2	2.07	0.55
1:B:346:GLN:HG3	1:B:347:MET:H	1.71	0.55
1:B:243:ILE:O	1:B:246:THR:HG22	2.07	0.55
1:A:456:ILE:HB	1:A:460:LEU:HD13	1.89	0.54
1:C:211:VAL:HG12	1:C:213:ARG:HG3	1.88	0.54
1:C:64:VAL:O	1:C:68:VAL:HG23	2.06	0.54
1:A:148:ALA:HB1	1:A:380:PHE:CZ	2.41	0.54
1:C:113:PHE:O	1:C:117:ILE:HG23	2.06	0.54
1:B:183:SER:OG	1:B:339:ASN:HB3	2.07	0.54
1:C:126:ARG:HD2	1:C:131:ASP:HA	1.88	0.54
1:C:252:CYS:O	1:C:256:LEU:HG	2.08	0.54
1:C:275:SER:HB3	1:C:278:THR:OG1	2.08	0.54
1:C:308:ALA:O	1:C:312:LEU:HD13	2.07	0.54
1:A:287:THR:HA	1:A:290:PHE:HB3	1.90	0.54
1:C:92:LEU:HD13	1:C:520:ASN:HD22	1.73	0.54
1:A:224:LEU:HD12	1:A:539:ALA:HB2	1.89	0.54
1:B:130:ILE:HD13	1:B:131:ASP:N	2.22	0.54
1:B:134:PRO:O	1:B:135:GLU:CB	2.56	0.54
1:B:153:ASP:O	1:B:156:PHE:N	2.41	0.54
1:B:519:GLN:HE21	1:B:520:ASN:ND2	2.06	0.54
1:B:534:ILE:O	1:B:537:MET:HB3	2.08	0.54
1:A:141:TRP:CD1	1:A:388:ILE:HG13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LYS:HA	1:C:302:ILE:H	1.72	0.54
1:C:380:PHE:HE2	4:C:601:CHT:H73	1.71	0.54
1:B:372:ALA:CB	1:B:523:ILE:HG23	2.38	0.54
1:A:366:TRP:O	1:A:369:PHE:HB3	2.07	0.54
1:B:451:GLN:CD	1:B:451:GLN:H	2.12	0.54
1:C:250:THR:HG22	1:C:377:TRP:HE1	1.73	0.54
1:B:309:ASN:ND2	1:B:464:PHE:HB3	2.24	0.53
1:A:527:THR:N	1:A:528:PRO:CD	2.71	0.53
1:C:305:LEU:HA	1:C:308:ALA:HB3	1.89	0.53
1:A:156:PHE:CE2	1:A:256:LEU:HD11	2.44	0.53
1:A:235:GLY:H	1:A:238:ILE:HD13	1.73	0.53
1:A:325:PRO:HB2	1:A:328:SER:HB2	1.91	0.53
3:A:602:PGT:C23	1:C:399:LEU:HD21	2.38	0.53
1:B:108:THR:OG1	1:B:192:HIS:HE1	1.91	0.53
1:C:380:PHE:CE1	1:C:471:SER:HB2	2.43	0.53
1:B:114:ILE:HG23	1:B:199:ILE:HD12	1.88	0.53
1:B:123:GLY:HA2	1:B:394:ILE:CD1	2.39	0.53
1:B:213:ARG:NH1	1:B:222:VAL:HB	2.24	0.53
1:B:435:ALA:O	1:B:438:GLU:HG2	2.08	0.53
1:B:150:MET:CE	1:B:154:LEU:HD23	2.37	0.53
1:B:260:GLN:CG	1:B:461:LEU:HD13	2.37	0.53
1:B:463:THR:O	1:B:464:PHE:CG	2.62	0.53
1:C:488:ASN:HB3	1:C:491:VAL:HG12	1.90	0.53
1:A:67:LEU:HA	1:A:70:VAL:HB	1.91	0.53
1:B:384:PHE:CE1	1:B:471:SER:HB2	2.43	0.53
1:A:375:ILE:HD13	1:A:530:LEU:HA	1.90	0.53
1:C:314:ALA:O	1:C:318:ILE:HG13	2.09	0.53
1:B:530:LEU:C	1:B:530:LEU:HD23	2.28	0.53
1:A:498:ALA:O	1:A:499:THR:HB	2.09	0.53
1:B:153:ASP:C	1:B:155:MET:N	2.58	0.53
1:C:152:ILE:HG21	1:C:253:SER:O	2.08	0.53
1:A:112:PHE:O	1:A:116:VAL:HG13	2.09	0.53
1:B:111:VAL:HG22	1:B:191:LEU:O	2.09	0.53
1:C:421:ILE:O	1:C:425:GLN:HG3	2.09	0.53
1:B:463:THR:O	1:B:465:PHE:N	2.38	0.52
1:C:81:LYS:O	1:C:82:ASP:HB3	2.09	0.52
1:C:170:VAL:HG13	1:C:171:PRO:HD2	1.92	0.52
1:A:88:ALA:CB	1:A:520:ASN:HD21	2.17	0.52
1:C:226:GLY:CA	1:C:227:GLU:CB	2.83	0.52
1:C:517:ASN:O	1:C:521:VAL:HG22	2.09	0.52
1:A:222:VAL:N	1:A:223:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LEU:HB3	1:B:467:THR:HG21	1.90	0.52
1:B:531:PHE:HA	1:B:534:ILE:HG12	1.91	0.52
1:C:250:THR:HG21	1:C:472:ALA:CB	2.38	0.52
1:A:107:GLY:HA2	1:A:110:PHE:CD2	2.45	0.52
1:A:376:SER:OG	1:A:526:ALA:HB3	2.09	0.52
1:C:191:LEU:HB2	1:C:340:TYR:OH	2.09	0.52
1:C:230:ALA:O	1:C:231:GLU:CB	2.56	0.52
1:A:150:MET:HE1	1:A:374:TRP:CZ3	2.42	0.52
1:A:316:LEU:HD13	1:A:416:PHE:HZ	1.73	0.52
1:C:529:PHE:O	1:C:530:LEU:C	2.48	0.52
1:A:292:PHE:HA	1:A:293:SER:C	2.29	0.52
1:B:187:PHE:CD1	1:B:347:MET:HG3	2.45	0.52
1:B:468:SER:O	1:B:472:ALA:HB2	2.10	0.52
1:C:67:LEU:HD23	1:C:70:VAL:HG11	1.91	0.52
1:B:298:VAL:O	1:B:298:VAL:CG1	2.54	0.52
1:B:371:TRP:CE3	1:B:374:TRP:HD1	2.27	0.52
1:C:385:LEU:HD22	1:C:401:VAL:HG22	1.91	0.52
1:A:392:ARG:HD2	1:A:396:GLU:CG	2.39	0.51
1:B:249:GLY:O	1:B:253:SER:OG	2.28	0.51
1:B:512:ASP:O	1:B:513:ASN:HB2	2.08	0.51
1:A:101:TRP:CE2	1:C:330:LEU:HD13	2.44	0.51
1:B:76:TRP:O	1:B:85:THR:HB	2.09	0.51
1:B:204:ILE:HD11	1:B:217:LEU:HA	1.93	0.51
1:B:279:ILE:O	1:B:283:VAL:HB	2.10	0.51
1:C:94:ALA:O	1:C:98:ASN:OD1	2.28	0.51
1:A:254:LEU:HD22	1:A:465:PHE:CZ	2.45	0.51
1:A:515:LEU:N	1:A:515:LEU:CD1	2.73	0.51
1:A:74:VAL:HG13	1:A:502:ILE:HB	1.93	0.51
1:B:260:GLN:HG2	1:B:461:LEU:HD22	1.93	0.51
1:A:318:ILE:O	1:A:322:VAL:HG22	2.10	0.51
1:A:506:LEU:C	1:A:506:LEU:CD2	2.76	0.51
1:A:149:GLY:HA2	1:A:381:VAL:CG1	2.41	0.51
1:A:156:PHE:CD2	1:A:256:LEU:HD11	2.46	0.51
1:A:352:ALA:HB3	1:C:331:ASN:ND2	2.26	0.51
1:B:103:PHE:HE1	1:B:372:ALA:HA	1.75	0.51
1:B:128:GLY:HA2	1:B:209:PHE:O	2.10	0.51
1:B:364:GLY:HA2	1:B:368:ILE:HB	1.91	0.51
1:C:67:LEU:HA	1:C:70:VAL:CG1	2.38	0.51
1:A:112:PHE:HZ	1:A:345:PHE:CZ	2.29	0.51
1:A:393:SER:HB3	1:A:396:GLU:CG	2.41	0.51
1:A:568:ARG:HH11	1:C:552:GLU:HG3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ILE:HG22	1:C:226:GLY:O	2.10	0.51
1:A:160:THR:O	1:A:164:THR:HG22	2.11	0.51
1:C:404:VAL:CB	1:C:405:PRO:HD3	2.39	0.51
1:A:74:VAL:O	1:A:78:ILE:HG22	2.11	0.51
1:B:374:TRP:HA	1:B:374:TRP:CE3	2.46	0.51
1:C:551:LEU:O	1:C:555:GLU:HG3	2.10	0.51
1:A:186:MET:HE3	1:A:190:THR:HG21	1.92	0.50
1:A:222:VAL:HB	1:A:227:GLU:HA	1.92	0.50
1:B:96:VAL:HG13	1:B:368:ILE:HG21	1.92	0.50
1:C:234:LEU:O	1:C:236:LYS:N	2.44	0.50
1:A:121:LYS:CG	3:A:602:PGT:H11	2.41	0.50
1:A:142:ILE:H	1:A:142:ILE:CD1	2.23	0.50
1:A:331:ASN:O	1:A:334:PRO:HD2	2.10	0.50
1:B:99:LEU:O	1:B:103:PHE:HD2	1.93	0.50
1:B:196:ILE:HD11	1:B:374:TRP:CB	2.27	0.50
1:B:375:ILE:HG12	1:B:530:LEU:HA	1.92	0.50
1:C:524:VAL:O	1:C:528:PRO:HD3	2.11	0.50
1:A:136:PHE:O	1:A:137:ARG:CB	2.59	0.50
1:A:292:PHE:HA	1:A:293:SER:O	2.11	0.50
1:A:63:ILE:O	1:A:66:ALA:HB3	2.11	0.50
1:B:70:VAL:O	1:B:74:VAL:HG12	2.11	0.50
1:B:227:GLU:C	1:B:229:GLY:H	2.15	0.50
1:C:76:TRP:HB2	5:C:709:HOH:O	2.11	0.50
1:A:101:TRP:CZ2	1:C:330:LEU:HD13	2.46	0.50
1:A:221:PHE:O	1:A:225:ILE:HG12	2.12	0.50
1:B:232:GLY:O	1:B:233:TRP:C	2.49	0.50
1:B:176:HIS:N	1:B:176:HIS:CD2	2.79	0.50
1:B:206:TYR:O	1:B:210:ARG:HB3	2.11	0.50
1:C:129:ARG:NH1	1:C:130:ILE:H	2.09	0.50
1:A:81:LYS:HB3	1:A:84:PHE:HB2	1.94	0.50
1:A:115:VAL:HG11	3:A:602:PGT:H421	1.93	0.50
1:A:139:VAL:HG23	1:A:140:SER:N	2.27	0.50
1:A:273:ASP:HB3	1:A:274:PRO:CD	2.39	0.50
1:C:75:VAL:HG12	1:C:76:TRP:N	2.26	0.50
1:A:269:ASN:OD1	1:A:271:ILE:HG13	2.11	0.49
1:A:451:GLN:O	1:A:455:ILE:HG13	2.10	0.49
1:B:458:MET:HA	1:B:461:LEU:CD1	2.36	0.49
1:A:161:GLU:HB3	1:A:162:PRO:HD3	1.93	0.49
1:A:330:LEU:HG	1:B:101:TRP:CG	2.47	0.49
1:B:250:THR:O	1:B:254:LEU:HG	2.12	0.49
1:B:354:SER:O	1:B:359:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ILE:HG13	1:B:456:ILE:N	2.26	0.49
1:B:540:LEU:O	1:B:544:LEU:HG	2.11	0.49
1:A:222:VAL:HB	1:A:227:GLU:HG2	1.94	0.49
1:B:121:LYS:NZ	1:B:550:TYR:HD1	2.10	0.49
1:B:185:THR:O	1:B:189:TRP:HD1	1.96	0.49
1:C:106:PHE:HA	1:C:109:VAL:HB	1.94	0.49
1:B:129:ARG:O	1:B:130:ILE:HG22	2.13	0.49
1:C:66:ALA:N	1:C:240:ILE:HD11	2.27	0.49
1:C:284:SER:HA	1:C:287:THR:CG2	2.36	0.49
1:A:455:ILE:HG23	1:A:459:ILE:HD12	1.95	0.49
3:A:602:PGT:O31	3:A:602:PGT:H12	2.11	0.49
1:C:520:ASN:O	1:C:524:VAL:HG23	2.12	0.49
1:A:156:PHE:HE1	1:A:437:GLU:HG3	1.78	0.49
1:B:281:GLY:C	1:B:282:ILE:HD12	2.32	0.49
1:C:78:ILE:HG13	1:C:79:GLY:N	2.28	0.49
1:B:234:LEU:HD12	1:B:234:LEU:N	2.28	0.49
1:A:159:THR:OG1	1:A:443:LEU:HD21	2.12	0.49
1:A:373:TRP:HE1	1:A:377:TRP:HE3	1.60	0.49
1:B:89:SER:O	1:B:92:LEU:HB3	2.12	0.49
1:B:305:LEU:HB3	1:B:467:THR:CG2	2.43	0.49
1:A:430:ILE:HG13	1:A:443:LEU:HB3	1.95	0.49
1:B:399:LEU:HD12	1:B:399:LEU:C	2.33	0.49
1:C:449:GLY:O	1:C:452:ILE:HG12	2.13	0.49
1:A:325:PRO:HD2	1:A:419:THR:HG22	1.95	0.48
1:C:316:LEU:O	1:C:320:VAL:HG23	2.13	0.48
1:A:70:VAL:O	1:A:74:VAL:HG23	2.13	0.48
1:A:138:THR:HG23	1:A:139:VAL:HG13	1.95	0.48
1:A:378:SER:HA	1:A:381:VAL:CG2	2.43	0.48
1:C:156:PHE:CE1	1:C:256:LEU:HB2	2.48	0.48
1:C:76:TRP:CD1	1:C:76:TRP:C	2.86	0.48
1:C:430:ILE:HG21	1:C:443:LEU:HA	1.96	0.48
1:B:186:MET:HE1	1:B:336:SER:HB3	1.95	0.48
1:C:375:ILE:HD11	1:C:530:LEU:HD13	1.94	0.48
1:C:431:TRP:NE1	1:C:434:GLY:HA2	2.28	0.48
1:A:370:TYR:C	1:A:374:TRP:CD1	2.87	0.48
1:A:380:PHE:CD1	1:A:472:ALA:HA	2.48	0.48
1:A:497:VAL:O	1:A:499:THR:N	2.45	0.48
1:B:141:TRP:HD1	1:B:145:MET:SD	2.36	0.48
1:C:112:PHE:O	1:C:113:PHE:C	2.52	0.48
1:C:323:VAL:HG22	1:C:447:LEU:HD22	1.95	0.48
1:A:456:ILE:HB	1:A:460:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:TYR:CE1	1:B:210:ARG:HG2	2.48	0.48
1:A:128:GLY:O	1:A:129:ARG:C	2.51	0.48
1:A:150:MET:CE	1:A:374:TRP:HZ3	2.23	0.48
1:A:499:THR:O	1:A:503:GLY:N	2.47	0.48
1:B:316:LEU:O	1:B:319:PHE:HB3	2.14	0.48
1:B:467:THR:HA	1:B:470:ASP:OD2	2.14	0.48
1:C:311:VAL:O	1:C:315:LEU:HD13	2.14	0.48
1:C:554:ARG:HD3	1:C:557:GLN:HE21	1.79	0.48
1:A:95:VAL:HG23	1:A:96:VAL:N	2.29	0.48
1:A:473:SER:HA	1:A:476:MET:HG2	1.96	0.48
1:A:162:PRO:HG2	1:A:417:GLY:HA3	1.96	0.47
1:B:194:TRP:CE3	1:B:197:TYR:HD2	2.32	0.47
1:B:476:MET:HA	1:B:479:MET:HG2	1.96	0.47
1:B:519:GLN:HA	5:B:608:HOH:O	2.14	0.47
1:B:325:PRO:HB2	1:B:328:SER:HB2	1.95	0.47
1:A:94:ALA:O	1:A:98:ASN:HB2	2.14	0.47
1:A:188:HIS:HA	1:A:371:TRP:HH2	1.79	0.47
1:B:254:LEU:HA	1:B:465:PHE:CZ	2.49	0.47
1:A:570:HIS:O	1:A:574:ARG:HG2	2.14	0.47
1:A:78:ILE:HG12	1:A:505:THR:HB	1.95	0.47
1:B:373:TRP:O	1:B:376:SER:HB3	2.15	0.47
1:A:418:GLY:O	1:A:422:VAL:HG23	2.14	0.47
1:B:100:GLY:O	1:B:104:ILE:HG13	2.15	0.47
1:B:280:VAL:O	1:B:284:SER:HB3	2.15	0.47
1:B:371:TRP:HE3	1:B:374:TRP:HD1	1.61	0.47
1:B:443:LEU:HD12	1:B:443:LEU:O	2.14	0.47
1:C:117:ILE:HG13	1:C:118:ALA:N	2.29	0.47
1:C:471:SER:O	1:C:475:VAL:HG23	2.15	0.47
1:A:222:VAL:CG2	1:A:223:PRO:HD3	2.44	0.47
1:B:486:GLU:CD	1:B:486:GLU:H	2.18	0.47
1:A:194:TRP:CE3	1:A:197:TYR:HD2	2.33	0.47
1:A:287:THR:O	1:A:291:ILE:HG12	2.15	0.47
1:A:292:PHE:N	1:A:293:SER:CB	2.68	0.47
1:C:103:PHE:CZ	1:C:527:THR:HG22	2.50	0.47
1:C:162:PRO:CG	1:C:417:GLY:HA3	2.45	0.47
1:C:418:GLY:O	1:C:422:VAL:HG23	2.15	0.47
1:A:67:LEU:HD12	1:A:67:LEU:H	1.80	0.47
1:A:250:THR:O	1:A:254:LEU:HG	2.15	0.47
1:A:371:TRP:HA	1:A:374:TRP:HD1	1.80	0.47
1:A:515:LEU:HB3	1:A:516:SER:HA	1.96	0.47
1:B:276:ASP:O	1:B:278:THR:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD12	1:A:67:LEU:N	2.30	0.46
1:C:309:ASN:HD21	1:C:467:THR:HG21	1.80	0.46
1:B:136:PHE:HB3	1:B:140:SER:HB2	1.97	0.46
1:B:153:ASP:OD1	1:B:256:LEU:CD2	2.63	0.46
1:C:473:SER:HB3	1:C:492:THR:O	2.15	0.46
1:A:167:ARG:HG2	1:A:168:ASN:OD1	2.15	0.46
1:A:297:GLY:CA	1:A:298:VAL:HG22	2.46	0.46
1:B:112:PHE:O	1:B:116:VAL:HG23	2.15	0.46
1:C:415:ILE:O	1:C:419:THR:HG23	2.15	0.46
1:C:451:GLN:O	1:C:455:ILE:HG13	2.16	0.46
1:A:208:THR:HG21	1:A:215:GLN:CD	2.35	0.46
1:A:247:VAL:HG13	1:A:498:ALA:HB1	1.98	0.46
1:A:370:TYR:O	1:A:374:TRP:CD1	2.68	0.46
1:C:141:TRP:HD1	1:C:388:ILE:HG22	1.81	0.46
1:A:574:ARG:HA	1:A:577:GLU:HG2	1.98	0.46
1:B:151:GLY:O	1:B:155:MET:HG3	2.15	0.46
1:B:430:ILE:HD12	1:B:430:ILE:O	2.16	0.46
1:C:377:TRP:C	1:C:379:PRO:HD2	2.35	0.46
1:A:88:ALA:HA	1:A:91:ALA:HB3	1.98	0.46
1:A:125:ILE:O	1:A:394:ILE:HG12	2.16	0.46
1:C:151:GLY:O	1:C:152:ILE:C	2.54	0.46
1:A:371:TRP:HE3	1:A:374:TRP:CD1	2.34	0.46
1:A:378:SER:N	1:A:379:PRO:CD	2.78	0.46
1:A:387:ARG:H	1:A:387:ARG:NE	2.13	0.46
1:B:58:LEU:HD21	1:B:481:GLN:HE21	1.80	0.46
1:B:314:ALA:O	1:B:318:ILE:HG13	2.16	0.46
1:B:322:VAL:HG23	1:B:323:VAL:N	2.30	0.46
1:C:211:VAL:CG1	1:C:213:ARG:HG3	2.46	0.46
1:C:475:VAL:HG12	1:C:479:MET:HE2	1.98	0.46
1:A:243:ILE:O	1:A:247:VAL:HG23	2.15	0.46
1:B:150:MET:HE2	1:B:154:LEU:CD2	2.41	0.46
1:B:354:SER:HA	1:B:355:ALA:HA	1.71	0.46
1:B:377:TRP:O	1:B:381:VAL:HG23	2.16	0.46
1:A:292:PHE:CA	1:A:293:SER:C	2.84	0.46
1:A:346:GLN:O	1:A:346:GLN:HG2	2.16	0.46
1:B:344:PHE:O	1:B:348:ALA:HB2	2.16	0.46
1:A:188:HIS:HA	1:A:371:TRP:CH2	2.51	0.45
1:A:512:ASP:O	1:A:513:ASN:HB3	2.15	0.45
1:B:142:ILE:HG23	1:B:310:MET:SD	2.56	0.45
1:C:159:THR:HG22	1:C:416:PHE:HB3	1.98	0.45
1:C:210:ARG:HH22	1:C:549:ILE:CG1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:THR:HG21	1:C:472:ALA:HB1	1.97	0.45
1:B:139:VAL:HG12	1:B:139:VAL:O	2.16	0.45
1:A:178:VAL:O	1:A:182:MET:HG2	2.16	0.45
1:A:332:LEU:O	1:A:332:LEU:HD23	2.17	0.45
1:B:71:LEU:HD23	1:B:71:LEU:O	2.16	0.45
1:B:476:MET:CE	1:B:495:TRP:HE3	2.30	0.45
1:C:414:SER:O	1:C:418:GLY:HA3	2.15	0.45
1:A:105:LEU:O	1:A:109:VAL:HG23	2.17	0.45
1:A:302:ILE:HG23	1:A:305:LEU:HD21	1.99	0.45
1:A:378:SER:N	1:A:379:PRO:HD2	2.31	0.45
1:A:444:LEU:HD12	1:A:445:HIS:N	2.31	0.45
1:A:108:THR:HA	1:A:192:HIS:NE2	2.32	0.45
1:A:323:VAL:HG12	1:A:447:LEU:HD22	1.97	0.45
1:C:503:GLY:O	1:C:507:LEU:HD13	2.16	0.45
1:C:225:ILE:CG2	1:C:226:GLY:N	2.79	0.45
1:C:428:GLU:OE1	1:C:428:GLU:N	2.49	0.45
1:A:269:ASN:O	1:A:271:ILE:HB	2.16	0.45
1:A:301:GLY:CA	1:A:302:ILE:C	2.85	0.45
1:A:333:LEU:HB3	1:A:334:PRO:HD3	1.99	0.45
1:A:393:SER:HB3	1:A:396:GLU:HG2	1.98	0.45
1:B:141:TRP:CZ2	1:B:389:SER:HB3	2.50	0.45
1:B:547:ASP:OD1	1:B:548:VAL:HG22	2.16	0.45
1:A:159:THR:HG21	1:A:440:LEU:HA	1.99	0.45
1:A:558:ARG:HH11	1:A:558:ARG:HA	1.82	0.45
1:B:300:LYS:CG	1:B:303:GLN:HB2	2.45	0.45
1:B:374:TRP:HA	1:B:374:TRP:HE3	1.81	0.45
1:C:60:TRP:C	1:C:62:VAL:H	2.20	0.45
1:C:417:GLY:O	1:C:421:ILE:HG12	2.17	0.45
1:A:57:SER:HB2	1:A:482:HIS:ND1	2.32	0.44
1:A:343:ASN:O	1:A:347:MET:HG3	2.16	0.44
1:A:385:LEU:HD21	1:A:401:VAL:CG2	2.43	0.44
1:B:103:PHE:CE1	1:B:372:ALA:HA	2.52	0.44
1:B:161:GLU:HG2	1:B:185:THR:OG1	2.16	0.44
1:B:373:TRP:CD1	1:B:373:TRP:C	2.88	0.44
1:C:91:ALA:O	1:C:94:ALA:HB3	2.17	0.44
1:A:107:GLY:O	1:A:110:PHE:HB2	2.17	0.44
1:A:139:VAL:HG23	1:A:140:SER:H	1.82	0.44
1:C:375:ILE:CD1	1:C:530:LEU:HD13	2.47	0.44
1:B:193:PRO:HG3	1:B:374:TRP:NE1	2.31	0.44
1:B:505:THR:HA	1:B:508:LEU:HG	1.99	0.44
1:C:208:THR:HG21	1:C:215:GLN:CG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:VAL:HG23	1:C:179:GLY:N	2.32	0.44
1:C:244:ILE:HG23	1:C:248:PHE:HE2	1.83	0.44
1:A:127:LEU:HD12	1:A:392:ARG:O	2.18	0.44
1:B:92:LEU:CD1	1:B:523:ILE:HG21	2.48	0.44
1:B:189:TRP:CZ2	1:B:370:TYR:OH	2.69	0.44
1:B:240:ILE:O	1:B:244:ILE:HG13	2.16	0.44
1:B:371:TRP:CE3	1:B:371:TRP:HA	2.52	0.44
1:B:371:TRP:HE3	1:B:371:TRP:HA	1.82	0.44
1:C:82:ASP:O	1:C:85:THR:HG22	2.16	0.44
1:C:259:LEU:HD13	1:C:437:GLU:OE1	2.18	0.44
1:A:101:TRP:CG	1:A:102:ALA:N	2.85	0.44
1:C:476:MET:HA	1:C:479:MET:HE2	2.00	0.44
1:C:527:THR:N	1:C:528:PRO:CD	2.81	0.44
1:A:223:PRO:HG2	1:A:543:ASP:HB2	1.99	0.44
1:A:333:LEU:HB3	1:A:334:PRO:CD	2.47	0.44
1:A:514:ALA:C	1:A:515:LEU:HD12	2.37	0.44
1:B:151:GLY:O	1:B:155:MET:CG	2.66	0.44
1:C:74:VAL:HG12	1:C:505:THR:OG1	2.18	0.44
1:C:159:THR:CG2	1:C:416:PHE:HB3	2.48	0.44
1:C:225:ILE:O	1:C:227:GLU:HB2	2.18	0.44
1:A:146:PHE:O	1:A:147:ALA:C	2.56	0.44
1:A:167:ARG:NH1	1:A:431:TRP:CG	2.85	0.44
1:A:381:VAL:O	1:A:385:LEU:HB2	2.17	0.44
1:C:62:VAL:C	1:C:65:PRO:HD2	2.38	0.44
1:C:99:LEU:HD11	1:C:531:PHE:HZ	1.82	0.44
1:C:187:PHE:HA	1:C:340:TYR:HE1	1.83	0.44
1:C:206:TYR:CE2	1:C:211:VAL:HG23	2.53	0.44
1:A:92:LEU:HD12	1:A:92:LEU:C	2.39	0.44
1:A:204:ILE:HD11	1:A:217:LEU:HD12	2.00	0.44
1:B:106:PHE:HB3	1:B:110:PHE:CZ	2.53	0.44
1:C:141:TRP:CD1	1:C:388:ILE:HG22	2.53	0.44
1:C:371:TRP:HA	1:C:371:TRP:CE3	2.53	0.44
1:A:540:LEU:HD22	1:A:544:LEU:HD22	2.00	0.43
1:B:186:MET:CE	1:B:336:SER:HB3	2.48	0.43
1:B:276:ASP:O	1:B:277:TRP:CD1	2.71	0.43
1:C:114:ILE:HD12	1:C:114:ILE:HA	1.81	0.43
1:A:461:LEU:O	1:A:461:LEU:HD12	2.18	0.43
1:B:95:VAL:HG23	1:B:99:LEU:HD12	2.00	0.43
1:B:141:TRP:O	1:B:142:ILE:C	2.56	0.43
1:B:149:GLY:O	1:B:150:MET:HG3	2.18	0.43
1:B:549:ILE:HD12	1:B:550:TYR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:OE2	1:C:390:ARG:HG2	2.18	0.43
1:C:138:THR:O	1:C:142:ILE:HG13	2.18	0.43
1:C:217:LEU:HD12	1:C:242:ALA:HB2	2.00	0.43
3:A:602:PGT:H232	1:C:399:LEU:HD21	2.00	0.43
1:B:81:LYS:HZ2	1:B:84:PHE:HD2	1.67	0.43
1:C:193:PRO:O	1:C:196:ILE:HB	2.18	0.43
1:A:199:ILE:HG22	1:A:536:LEU:HD23	2.00	0.43
1:A:497:VAL:O	1:A:498:ALA:C	2.56	0.43
1:C:173:HIS:CD2	1:C:180:VAL:HG11	2.53	0.43
1:A:189:TRP:CZ3	1:A:374:TRP:HH2	2.37	0.43
1:A:481:GLN:O	1:A:484:GLN:HG2	2.18	0.43
1:A:536:LEU:O	1:A:540:LEU:HB2	2.18	0.43
1:B:64:VAL:O	1:B:68:VAL:HG22	2.18	0.43
1:B:256:LEU:HD13	1:B:256:LEU:O	2.18	0.43
1:C:124:THR:HG23	1:C:395:ARG:HH21	1.83	0.43
1:C:371:TRP:CE3	1:C:371:TRP:CA	3.02	0.43
1:A:115:VAL:CG1	3:A:602:PGT:H402	2.48	0.43
1:B:157:TYR:HD1	1:B:160:THR:CG2	2.31	0.43
1:B:233:TRP:HB2	1:B:234:LEU:HD12	2.00	0.43
1:B:271:ILE:HG12	1:B:272:GLU:CA	2.49	0.43
1:A:112:PHE:HZ	1:A:345:PHE:CE1	2.37	0.43
1:A:331:ASN:HD22	1:B:352:ALA:HB3	1.82	0.43
1:B:243:ILE:HA	1:B:246:THR:HG22	2.00	0.43
1:B:256:LEU:HA	1:B:259:LEU:HG	2.00	0.43
1:B:271:ILE:CB	1:B:272:GLU:HA	2.47	0.43
1:C:67:LEU:CA	1:C:70:VAL:HG12	2.42	0.43
1:A:156:PHE:O	1:A:156:PHE:CG	2.71	0.43
1:A:292:PHE:H	1:A:293:SER:CB	2.07	0.43
1:B:143:SER:HB3	1:B:310:MET:SD	2.59	0.43
1:A:473:SER:HA	1:A:476:MET:SD	2.59	0.43
1:B:74:VAL:CG2	1:B:502:ILE:HB	2.49	0.43
1:C:216:LEU:HD21	1:C:483:GLY:N	2.34	0.43
1:C:239:ASP:O	1:C:243:ILE:HG12	2.19	0.43
1:C:540:LEU:O	1:C:544:LEU:HG	2.19	0.43
1:A:147:ALA:HB2	1:A:309:ASN:ND2	2.34	0.43
1:A:194:TRP:CZ2	1:A:405:PRO:HB3	2.54	0.43
1:A:445:HIS:HA	1:A:450:GLY:CA	2.38	0.43
1:C:103:PHE:HZ	1:C:527:THR:HG22	1.84	0.43
1:C:106:PHE:CD1	1:C:534:ILE:HD13	2.54	0.43
1:C:247:VAL:HG12	1:C:502:ILE:CD1	2.49	0.43
1:A:92:LEU:C	1:A:94:ALA:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:HB	1:A:406:ALA:HB1	2.00	0.42
1:A:232:GLY:O	1:A:233:TRP:C	2.56	0.42
1:A:505:THR:HA	1:A:508:LEU:CG	2.43	0.42
1:A:563:LEU:HD23	1:A:563:LEU:C	2.39	0.42
1:B:127:LEU:O	1:B:127:LEU:HG	2.19	0.42
1:C:521:VAL:HG23	1:C:522:THR:N	2.33	0.42
1:C:546:ASN:O	1:C:551:LEU:HD12	2.19	0.42
1:A:443:LEU:HD12	1:A:443:LEU:C	2.38	0.42
1:B:141:TRP:HH2	1:B:389:SER:CB	2.30	0.42
1:B:254:LEU:CD2	1:B:465:PHE:CE1	2.85	0.42
1:C:316:LEU:HB3	1:C:416:PHE:HZ	1.84	0.42
1:C:359:ALA:O	1:C:363:LEU:HG	2.18	0.42
1:C:506:LEU:HD23	1:C:518:LEU:HA	2.00	0.42
1:A:182:MET:CE	1:A:332:LEU:HD21	2.49	0.42
1:A:194:TRP:CE2	1:A:405:PRO:HB3	2.55	0.42
1:A:197:TYR:CD1	1:A:381:VAL:HG21	2.53	0.42
1:A:502:ILE:HA	1:A:505:THR:OG1	2.18	0.42
1:A:559:PHE:O	1:A:560:ASN:C	2.57	0.42
1:B:141:TRP:O	1:B:143:SER:N	2.52	0.42
1:B:463:THR:C	1:B:465:PHE:N	2.71	0.42
1:C:60:TRP:O	1:C:64:VAL:HG12	2.19	0.42
1:A:214:LYS:H	1:A:214:LYS:HG2	1.62	0.42
1:A:214:LYS:HG3	1:A:219:SER:OG	2.19	0.42
1:A:222:VAL:HG22	1:A:223:PRO:HD3	2.01	0.42
1:A:290:PHE:CE2	1:A:291:ILE:HG23	2.54	0.42
1:A:371:TRP:HA	1:A:371:TRP:CE3	2.54	0.42
1:B:158:GLY:HA2	1:B:413:PHE:CE1	2.54	0.42
1:B:189:TRP:HZ2	1:B:370:TYR:OH	2.02	0.42
1:B:331:ASN:HD22	1:C:352:ALA:HB3	1.84	0.42
1:C:154:LEU:HD23	1:C:413:PHE:CE2	2.54	0.42
1:C:303:GLN:HA	1:C:306:SER:HB3	2.01	0.42
1:C:330:LEU:HD23	1:C:330:LEU:HA	1.89	0.42
1:C:337:ILE:O	1:C:341:LEU:HG	2.20	0.42
1:C:353:MET:O	1:C:357:GLY:N	2.49	0.42
1:C:475:VAL:HG12	1:C:479:MET:CE	2.49	0.42
1:A:208:THR:HG21	1:A:215:GLN:HA	2.01	0.42
1:A:291:ILE:O	1:A:292:PHE:HB2	2.20	0.42
1:A:303:GLN:C	1:A:305:LEU:H	2.23	0.42
1:B:199:ILE:HG22	1:B:200:VAL:N	2.34	0.42
1:C:78:ILE:CG2	1:C:505:THR:HG23	2.41	0.42
1:C:108:THR:CA	1:C:192:HIS:CE1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:VAL:HG12	1:C:421:ILE:HG21	2.02	0.42
1:C:378:SER:N	1:C:379:PRO:CD	2.80	0.42
1:A:66:ALA:HB1	1:A:243:ILE:HD13	2.01	0.42
1:B:286:LEU:HD23	1:B:465:PHE:CD2	2.55	0.42
1:A:148:ALA:HB1	1:A:380:PHE:HZ	1.84	0.42
1:B:443:LEU:HD12	1:B:443:LEU:C	2.40	0.42
1:C:145:MET:CE	1:C:404:VAL:HG21	2.50	0.42
1:A:279:ILE:HG22	1:A:279:ILE:O	2.19	0.42
1:B:222:VAL:HB	1:B:223:PRO:HD3	2.00	0.42
1:B:233:TRP:CD1	1:B:233:TRP:N	2.84	0.42
1:C:81:LYS:HB3	1:C:84:PHE:HD2	1.80	0.42
1:C:166:TYR:CE2	1:C:176:HIS:HD2	2.38	0.42
1:C:527:THR:OG1	1:C:528:PRO:HD3	2.20	0.42
1:A:67:LEU:HD11	1:A:495:TRP:CH2	2.55	0.42
1:A:310:MET:O	1:A:311:VAL:C	2.58	0.42
1:A:369:PHE:CD1	1:A:369:PHE:C	2.93	0.42
1:B:104:ILE:HD12	1:B:105:LEU:N	2.35	0.42
1:B:152:ILE:HA	1:B:464:PHE:CZ	2.55	0.42
1:B:234:LEU:H	1:B:234:LEU:CD1	2.32	0.42
1:B:288:LEU:HA	1:B:291:ILE:HG22	2.00	0.42
1:B:321:PHE:HA	1:B:329:ILE:CD1	2.50	0.42
1:C:377:TRP:CH2	4:C:601:CHT:HC51	2.54	0.42
1:A:243:ILE:HD12	1:A:244:ILE:HG13	2.01	0.42
1:A:305:LEU:HD22	1:A:467:THR:HA	2.02	0.42
1:B:68:VAL:HG23	1:B:69:ILE:N	2.35	0.42
1:B:264:GLY:HA3	1:B:458:MET:SD	2.60	0.42
1:B:319:PHE:O	1:B:323:VAL:HG22	2.20	0.42
1:C:284:SER:CA	1:C:287:THR:HG22	2.41	0.42
1:A:456:ILE:HB	1:A:460:LEU:CD1	2.49	0.41
1:A:568:ARG:HH11	1:C:552:GLU:CG	2.33	0.41
1:B:213:ARG:HH11	1:B:222:VAL:HB	1.85	0.41
1:A:197:TYR:OH	1:A:374:TRP:HE3	2.03	0.41
1:B:302:ILE:HD11	1:B:474:THR:HG21	2.02	0.41
1:B:481:GLN:HE22	1:B:488:ASN:HB2	1.84	0.41
1:C:564:ALA:HA	1:C:567:ARG:HG2	2.02	0.41
1:A:78:ILE:HD13	1:A:505:THR:O	2.21	0.41
1:A:204:ILE:O	1:A:208:THR:HG23	2.19	0.41
1:A:371:TRP:CE3	1:A:371:TRP:CA	3.03	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.82	0.41
3:A:602:PGT:H231	1:C:399:LEU:HD21	2.02	0.41
1:B:341:LEU:HD23	1:C:345:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:PRO:HA	1:C:391:GLY:HA3	2.02	0.41
1:A:59:ASN:O	1:A:63:ILE:HG22	2.20	0.41
1:A:105:LEU:O	1:A:105:LEU:HD12	2.21	0.41
1:A:481:GLN:OE1	1:A:484:GLN:HG3	2.21	0.41
1:B:395:ARG:C	1:B:397:PHE:H	2.23	0.41
1:A:170:VAL:CG1	1:A:171:PRO:HD2	2.49	0.41
1:A:384:PHE:HA	1:A:387:ARG:HD2	2.02	0.41
1:B:327:VAL:O	1:B:331:ASN:N	2.48	0.41
1:C:290:PHE:CZ	1:C:496:GLY:HA3	2.55	0.41
1:C:463:THR:O	1:C:467:THR:HG23	2.21	0.41
1:A:114:ILE:CD1	1:A:402:LEU:HD11	2.51	0.41
1:A:116:VAL:O	1:A:120:SER:N	2.52	0.41
1:A:136:PHE:HD1	1:A:388:ILE:HB	1.85	0.41
1:A:219:SER:O	1:A:222:VAL:HG13	2.20	0.41
1:A:240:ILE:O	1:A:243:ILE:HG13	2.21	0.41
1:A:458:MET:O	1:A:461:LEU:HG	2.19	0.41
1:B:144:MET:SD	1:B:384:PHE:HD2	2.44	0.41
1:B:214:LYS:HE2	1:B:214:LYS:HB3	1.87	0.41
1:B:371:TRP:CE3	1:B:374:TRP:CD1	3.08	0.41
1:B:473:SER:O	1:B:476:MET:HB2	2.21	0.41
1:C:323:VAL:HG13	1:C:324:GLY:N	2.35	0.41
1:A:158:GLY:HA2	1:A:413:PHE:CE1	2.53	0.41
1:A:189:TRP:CZ2	1:A:370:TYR:HE1	2.38	0.41
1:A:299:GLY:HA2	1:A:487:ALA:HB2	2.03	0.41
1:A:354:SER:HA	1:A:355:ALA:HA	1.71	0.41
1:A:484:GLN:HG2	1:A:484:GLN:H	1.70	0.41
1:B:432:GLY:C	1:B:434:GLY:H	2.23	0.41
1:C:88:ALA:O	1:C:91:ALA:HB3	2.21	0.41
1:C:210:ARG:NH2	1:C:549:ILE:HG12	2.35	0.41
1:C:325:PRO:HD2	1:C:419:THR:HG22	2.02	0.41
1:C:466:ILE:N	1:C:466:ILE:HD12	2.35	0.41
1:A:65:PRO:C	1:A:68:VAL:HG12	2.41	0.41
1:A:110:PHE:CZ	1:A:534:ILE:HD13	2.56	0.41
1:A:130:ILE:HB	1:A:131:ASP:H	1.65	0.41
1:A:170:VAL:HG22	1:A:362:TRP:CZ2	2.55	0.41
1:A:280:VAL:O	1:A:284:SER:HB2	2.20	0.41
1:A:327:VAL:HG21	1:B:98:ASN:OD1	2.21	0.41
1:C:124:THR:HG23	1:C:395:ARG:NH2	2.35	0.41
1:C:159:THR:HA	1:C:417:GLY:CA	2.50	0.41
1:C:290:PHE:CE2	1:C:496:GLY:HA3	2.56	0.41
1:C:323:VAL:HG13	1:C:447:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TRP:HA	1:A:63:ILE:HG22	2.03	0.41
1:A:81:LYS:HB2	1:A:84:PHE:CB	2.50	0.41
1:A:145:MET:CE	1:A:385:LEU:HD13	2.51	0.41
1:A:410:THR:HG23	1:A:411:VAL:N	2.35	0.41
1:A:415:ILE:O	1:A:419:THR:HG23	2.21	0.41
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.94	0.41
1:A:548:VAL:HG23	1:A:549:ILE:N	2.36	0.41
1:B:150:MET:HE3	1:B:154:LEU:CD2	2.48	0.41
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.87	0.41
1:B:460:LEU:CA	1:B:463:THR:HG22	2.48	0.41
1:B:466:ILE:O	1:B:470:ASP:HB3	2.21	0.41
1:B:476:MET:HE2	1:B:495:TRP:CE3	2.52	0.41
1:C:129:ARG:HH12	1:C:130:ILE:HG13	1.85	0.41
1:C:270:ILE:N	1:C:270:ILE:HD12	2.36	0.41
1:C:556:GLN:O	1:C:560:ASN:HB2	2.20	0.41
1:A:156:PHE:CD2	1:A:156:PHE:O	2.74	0.41
1:A:163:LEU:HD22	1:A:420:ALA:HB1	2.02	0.41
1:A:175:GLU:H	1:A:175:GLU:HG2	1.74	0.41
1:B:372:ALA:HB1	1:B:523:ILE:HG23	2.03	0.41
1:B:455:ILE:CG1	1:B:456:ILE:N	2.83	0.41
1:C:440:LEU:O	1:C:443:LEU:HB3	2.21	0.41
1:A:97:ASP:O	1:C:327:VAL:CG1	2.63	0.40
1:A:183:SER:C	1:A:347:MET:HE1	2.41	0.40
1:A:329:ILE:HD13	1:A:415:ILE:HG22	2.02	0.40
1:A:424:GLU:OE1	1:A:424:GLU:N	2.54	0.40
1:B:320:VAL:HG12	1:B:447:LEU:HD13	2.03	0.40
1:B:453:MET:O	1:B:456:ILE:HG12	2.21	0.40
1:C:329:ILE:HD11	1:C:419:THR:CG2	2.51	0.40
1:A:209:PHE:HE2	1:A:386:ALA:O	2.03	0.40
1:A:516:SER:C	1:A:518:LEU:H	2.24	0.40
1:B:320:VAL:HG12	1:B:447:LEU:CD1	2.51	0.40
1:C:453:MET:HA	1:C:456:ILE:HD12	2.03	0.40
1:B:175:GLU:CD	1:B:175:GLU:H	2.25	0.40
1:A:301:GLY:HA2	1:A:302:ILE:CB	2.41	0.40
1:B:58:LEU:CD2	1:B:481:GLN:HE21	2.35	0.40
1:B:81:LYS:NZ	1:B:84:PHE:HD2	2.20	0.40
1:B:207:SER:HA	1:B:213:ARG:HH21	1.86	0.40
1:B:475:VAL:HG22	1:B:479:MET:HE2	2.04	0.40
1:C:64:VAL:N	1:C:65:PRO:CD	2.85	0.40
1:C:371:TRP:N	1:C:371:TRP:HE3	2.20	0.40
1:A:184:THR:N	1:A:347:MET:HE1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HB2	1:A:214:LYS:H	1.72	0.40
1:A:316:LEU:HD11	1:A:412:TRP:HH2	1.87	0.40
1:A:444:LEU:O	1:A:450:GLY:HA2	2.21	0.40
1:B:122:PHE:CD1	1:B:544:LEU:HB3	2.57	0.40
1:B:147:ALA:O	1:B:468:SER:OG	2.23	0.40
1:B:330:LEU:HG	1:C:101:TRP:CE2	2.57	0.40
1:B:466:ILE:O	1:B:466:ILE:HD12	2.22	0.40
1:C:184:THR:HG22	1:C:188:HIS:CE1	2.57	0.40
1:C:213:ARG:HD2	1:C:219:SER:O	2.20	0.40
1:C:311:VAL:O	1:C:314:ALA:HB3	2.22	0.40
1:C:317:ALA:O	1:C:318:ILE:C	2.60	0.40
1:C:389:SER:O	1:C:390:ARG:C	2.58	0.40
1:C:536:LEU:O	1:C:540:LEU:HB2	2.22	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	524/566 (93%)	414 (79%)	90 (17%)	20 (4%)	3 19
1	B	497/566 (88%)	406 (82%)	76 (15%)	15 (3%)	4 24
1	C	501/566 (88%)	411 (82%)	81 (16%)	9 (2%)	8 35
All	All	1522/1698 (90%)	1231 (81%)	247 (16%)	44 (3%)	4 25

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	498	ALA
1	A	499	THR
1	A	513	ASN

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Mol	Chain	Res	Type
1	B	134	PRO
1	B	135	GLU
1	B	233	TRP
1	B	274	PRO
1	B	432	GLY
1	B	513	ASN
1	C	231	GLU
1	C	429	SER
1	A	131	ASP
1	A	139	VAL
1	A	157	TYR
1	A	274	PRO
1	A	292	PHE
1	A	294	ALA
1	A	302	ILE
1	B	130	ILE
1	B	142	ILE
1	B	154	LEU
1	B	190	THR
1	B	298	VAL
1	B	464	PHE
1	C	152	ILE
1	C	234	LEU
1	C	235	GLY
1	C	416	PHE
1	A	129	ARG
1	A	130	ILE
1	C	171	PRO
1	C	232	GLY
1	A	93	SER
1	A	135	GLU
1	A	291	ILE
1	A	388	ILE
1	B	225	ILE
1	A	271	ILE
1	A	379	PRO
1	A	298	VAL
1	B	152	ILE
1	B	379	PRO
1	C	532	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	412/443 (93%)	391 (95%)	21 (5%)	24 54
1	B	391/443 (88%)	351 (90%)	40 (10%)	7 27
1	C	397/443 (90%)	370 (93%)	27 (7%)	16 44
All	All	1200/1329 (90%)	1112 (93%)	88 (7%)	14 40

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	130	ILE
1	A	136	PHE
1	A	141	TRP
1	A	142	ILE
1	A	157	TYR
1	A	192	HIS
1	A	290	PHE
1	A	291	ILE
1	A	351	THR
1	A	353	MET
1	A	371	TRP
1	A	373	TRP
1	A	387	ARG
1	A	396	GLU
1	A	424	GLU
1	A	439	GLN
1	A	461	LEU
1	A	529	PHE
1	A	544	LEU
1	A	573	HIS
1	B	74	VAL
1	B	82	ASP
1	B	92	LEU
1	B	117	ILE
1	B	130	ILE

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Mol	Chain	Res	Type
1	B	131	ASP
1	B	137	ARG
1	B	150	MET
1	B	153	ASP
1	B	155	MET
1	B	186	MET
1	B	190	THR
1	B	248	PHE
1	B	253	SER
1	B	271	ILE
1	B	273	ASP
1	B	277	TRP
1	B	286	LEU
1	B	290	PHE
1	B	320	VAL
1	B	327	VAL
1	B	347	MET
1	B	369	PHE
1	B	370	TYR
1	B	371	TRP
1	B	374	TRP
1	B	383	MET
1	B	384	PHE
1	B	390	ARG
1	B	402	LEU
1	B	408	VAL
1	B	409	SER
1	B	443	LEU
1	B	461	LEU
1	B	466	ILE
1	B	467	THR
1	B	470	ASP
1	B	502	ILE
1	B	512	ASP
1	B	543	ASP
1	C	76	TRP
1	C	92	LEU
1	C	96	VAL
1	C	98	ASN
1	C	116	VAL
1	C	117	ILE
1	C	121	LYS

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Mol	Chain	Res	Type
1	C	126	ARG
1	C	160	THR
1	C	189	TRP
1	C	215	GLN
1	C	277	TRP
1	C	288	LEU
1	C	356	ASP
1	C	365	SER
1	C	367	THR
1	C	368	ILE
1	C	371	TRP
1	C	374	TRP
1	C	377	TRP
1	C	414	SER
1	C	433	ASP
1	C	439	GLN
1	C	443	LEU
1	C	481	GLN
1	C	543	ASP
1	C	553	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	HIS
1	A	439	GLN
1	A	481	GLN
1	A	520	ASN
1	A	556	GLN
1	A	560	ASN
1	B	176	HIS
1	B	192	HIS
1	B	215	GLN
1	B	269	ASN
1	B	343	ASN
1	B	426	ASN
1	B	445	HIS
1	B	481	GLN
1	B	519	GLN
1	C	176	HIS
1	C	192	HIS
1	C	331	ASN

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Mol	Chain	Res	Type
1	C	484	GLN
1	C	519	GLN
1	C	520	ASN
1	C	556	GLN
1	C	557	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	PGT	A	602	-	50,50,50	0.83	2 (4%)	53,56,56	1.10	3 (5%)
4	CHT	C	601	-	6,6,6	0.83	0	8,8,8	0.35	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
3	PGT	A	602	-	-	27/55/55/55	-
4	CHT	C	601	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	PGT	O2-C2	-2.85	1.39	1.46
3	A	602	PGT	O3-C3	-2.35	1.39	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	PGT	O2-C31-C32	4.32	120.81	111.50
3	A	602	PGT	O3-C3-C2	2.99	117.14	108.43
3	A	602	PGT	O3-C11-C12	2.25	118.97	111.91

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	PGT	C1-O3P-P-O1P
3	A	602	PGT	C1-O3P-P-O2P
3	A	602	PGT	C20-C21-C22-C23
3	A	602	PGT	C1-O3P-P-O4P
3	A	602	PGT	C31-C32-C33-C34
3	A	602	PGT	C16-C17-C18-C19
3	A	602	PGT	C4-C5-C6-O6
3	A	602	PGT	C40-C41-C42-C43
3	A	602	PGT	C39-C40-C41-C42
3	A	602	PGT	C11-C12-C13-C14
3	A	602	PGT	C32-C33-C34-C35
3	A	602	PGT	O5-C5-C6-O6
3	A	602	PGT	C18-C19-C20-C21
3	A	602	PGT	C19-C20-C21-C22
3	A	602	PGT	O2-C2-C3-O3
3	A	602	PGT	O3P-C1-C2-C3
3	A	602	PGT	O3P-C1-C2-O2
3	A	602	PGT	C4-O4P-P-O3P
3	A	602	PGT	C1-C2-C3-O3
3	A	602	PGT	C1-C2-O2-C31
3	A	602	PGT	C43-C44-C45-C46
3	A	602	PGT	C13-C14-C15-C16

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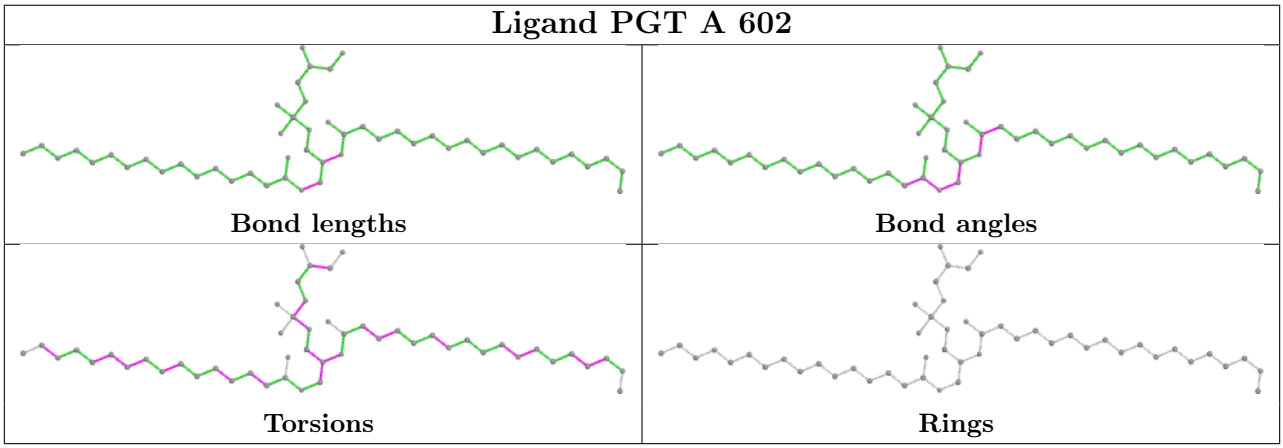
Mol	Chain	Res	Type	Atoms
3	A	602	PGT	C23-C24-C25-C26
3	A	602	PGT	C35-C36-C37-C38
3	A	602	PGT	C44-C45-C46-C47
3	A	602	PGT	C4-O4P-P-O1P
3	A	602	PGT	C3-C2-O2-C31

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PGT	10	0
4	C	601	CHT	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.



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	526/566 (92%)	0.46	51 (9%) 7 8	22, 120, 299, 416	0
1	B	501/566 (88%)	0.36	63 (12%) 3 3	13, 116, 284, 438	0
1	C	507/566 (89%)	-0.16	20 (3%) 39 36	9, 75, 181, 389	0
All	All	1534/1698 (90%)	0.22	134 (8%) 10 10	9, 98, 275, 438	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	ILE	19.9
1	A	299	GLY	16.7
1	C	81	LYS	12.9
1	A	513	ASN	10.6
1	A	294	ALA	9.3
1	B	512	ASP	8.1
1	A	505	THR	7.4
1	B	505	THR	7.3
1	B	508	LEU	7.1
1	A	509	SER	6.9
1	B	234	LEU	6.6
1	A	296	SER	6.6
1	A	298	VAL	6.4
1	B	550	TYR	6.4
1	A	227	GLU	6.0
1	A	506	LEU	5.9
1	A	304	TYR	5.9
1	B	504	LEU	5.8
1	A	516	SER	5.8
1	B	79	GLY	5.8
1	B	125	ILE	5.5
1	B	273	ASP	5.4
1	C	555	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	84	PHE	4.9
1	C	273	ASP	4.8
1	B	509	SER	4.8
1	C	568	ARG	4.8
1	A	517	ASN	4.7
1	A	508	LEU	4.4
1	A	274	PRO	4.4
1	C	274	PRO	4.4
1	B	551	LEU	4.3
1	A	512	ASP	4.2
1	C	270	ILE	4.1
1	B	225	ILE	4.1
1	A	268	ALA	3.9
1	A	80	PHE	3.8
1	A	504	LEU	3.8
1	A	501	ALA	3.8
1	A	137	ARG	3.7
1	B	80	PHE	3.7
1	A	273	ASP	3.7
1	B	275	SER	3.6
1	A	300	LYS	3.6
1	C	562	ARG	3.5
1	A	292	PHE	3.5
1	B	85	THR	3.5
1	B	556	GLN	3.5
1	B	252	CYS	3.4
1	A	234	LEU	3.4
1	B	297	GLY	3.4
1	A	252	CYS	3.4
1	A	81	LYS	3.3
1	B	391	GLY	3.3
1	A	254	LEU	3.3
1	C	79	GLY	3.3
1	A	136	PHE	3.3
1	B	490	TRP	3.3
1	B	251	ALA	3.3
1	B	390	ARG	3.3
1	B	127	LEU	3.2
1	C	296	SER	3.2
1	A	269	ASN	3.2
1	B	76	TRP	3.2
1	B	274	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	513	ASN	3.1
1	B	295	ILE	3.0
1	B	253	SER	3.0
1	A	279	ILE	3.0
1	B	151	GLY	3.0
1	B	510	GLY	3.0
1	B	129	ARG	3.0
1	B	272	GLU	2.9
1	B	141	TRP	2.9
1	C	174	ASP	2.9
1	A	447	LEU	2.9
1	A	228	LYS	2.9
1	B	552	GLU	2.8
1	A	60	TRP	2.8
1	B	396	GLU	2.8
1	C	80	PHE	2.7
1	B	501	ALA	2.7
1	B	393	SER	2.7
1	A	64	VAL	2.7
1	C	228	LYS	2.7
1	B	271	ILE	2.7
1	B	84	PHE	2.7
1	B	517	ASN	2.7
1	B	224	LEU	2.7
1	B	511	GLY	2.6
1	A	443	LEU	2.6
1	B	265	LEU	2.6
1	C	267	ALA	2.6
1	C	302	ILE	2.6
1	B	544	LEU	2.5
1	A	520	ASN	2.5
1	A	449	GLY	2.5
1	A	511	GLY	2.4
1	A	230	ALA	2.4
1	A	507	LEU	2.4
1	B	228	LYS	2.4
1	B	131	ASP	2.4
1	B	133	ALA	2.4
1	B	140	SER	2.4
1	A	485	LEU	2.3
1	C	554	ARG	2.3
1	A	84	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	145	MET	2.3
1	B	260	GLN	2.3
1	B	60	TRP	2.3
1	A	215	GLN	2.2
1	B	150	MET	2.2
1	A	514	ALA	2.2
1	C	58	LEU	2.2
1	B	255	GLY	2.2
1	B	557	GLN	2.2
1	B	128	GLY	2.2
1	B	146	PHE	2.2
1	B	303	GLN	2.2
1	B	250	THR	2.2
1	A	323	VAL	2.1
1	A	510	GLY	2.1
1	C	509	SER	2.1
1	B	555	GLU	2.1
1	A	388	ILE	2.1
1	A	253	SER	2.1
1	B	296	SER	2.1
1	A	145	MET	2.1
1	A	293	SER	2.1
1	C	229	GLY	2.1
1	B	298	VAL	2.0
1	B	545	SER	2.0
1	C	451	GLN	2.0
1	B	268	ALA	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,

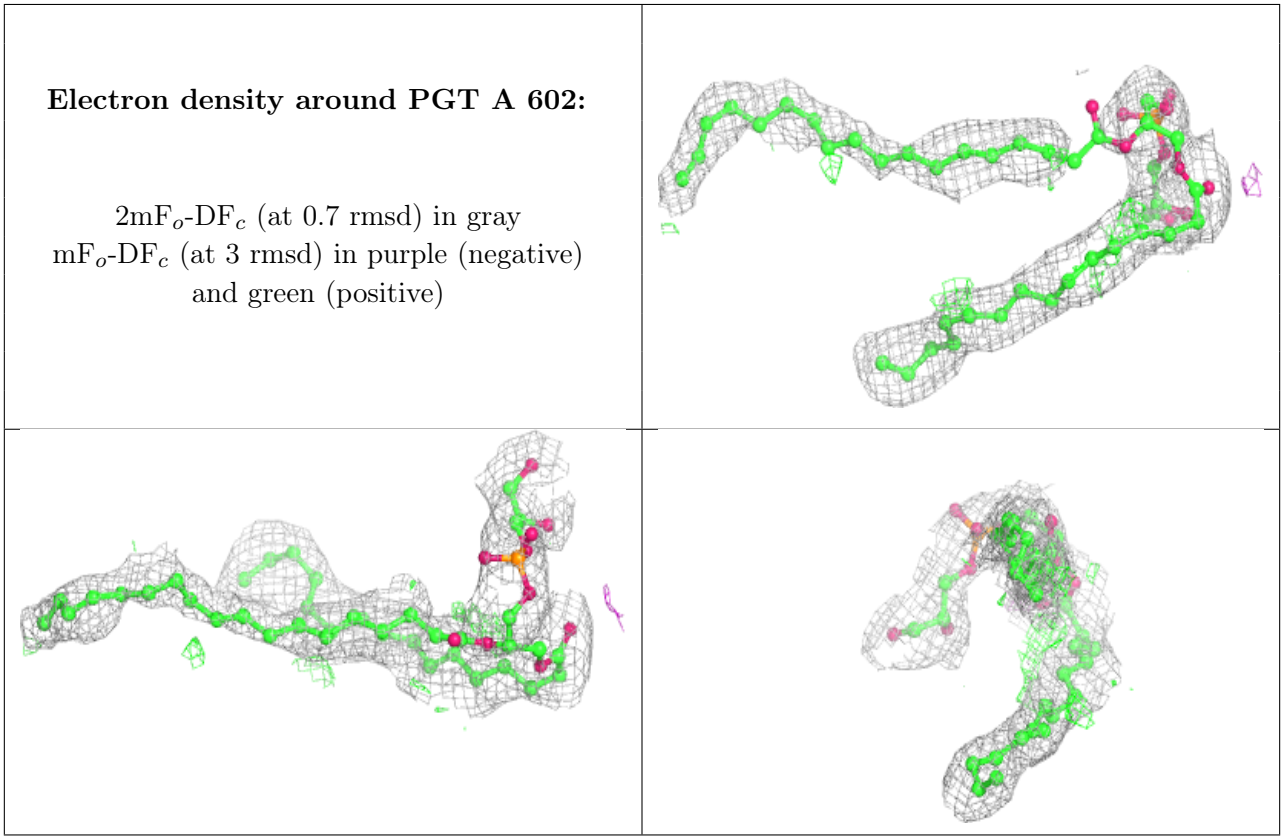
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGT	A	602	51/51	0.90	0.29	24,47,72,73	30
4	CHT	C	601	7/7	0.90	0.28	99,103,112,121	0
2	CL	A	601	1/1	0.94	0.19	105,105,105,105	0
2	CL	C	602	1/1	0.97	0.11	57,57,57,57	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 PGT A 602:

$2mF_o$-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

There are no such residues in this entry.