



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:51 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

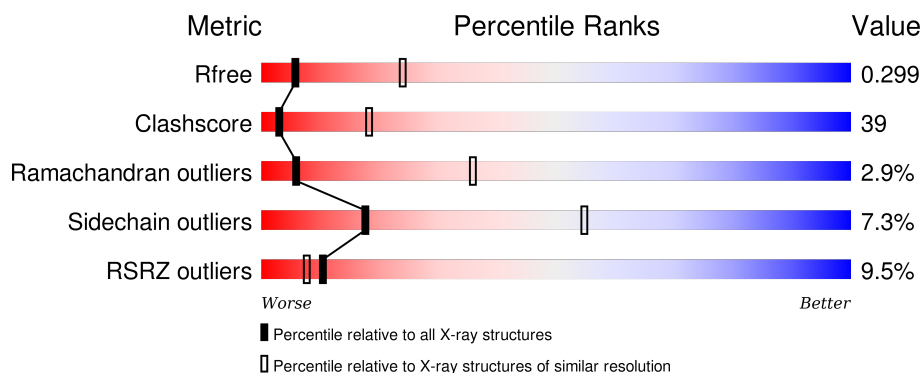
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>10%</div> <div>39% 48% 6% 7%</div> </div>
1	B	566	<div> <div>11%</div> <div>38% 42% 7% 11%</div> </div>
1	C	566	<div> <div>4%</div> <div>38% 48% • 10%</div> </div>

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
4	CHT	C	601	-	-	-	X

2 Entry composition

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			

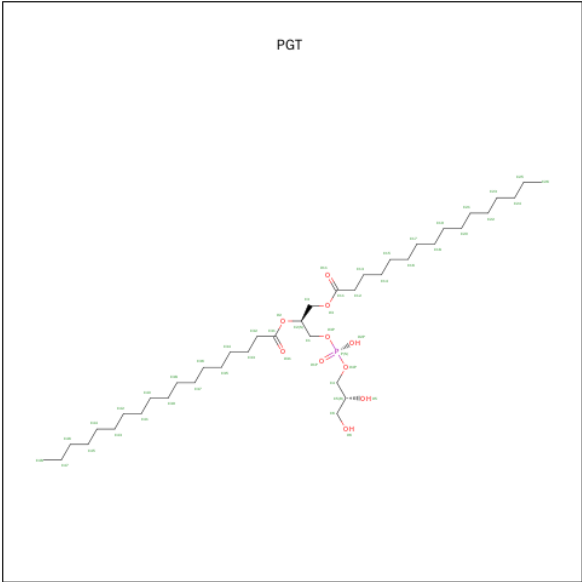
There are 3 discrepancies between the modelled and reference sequences:

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).

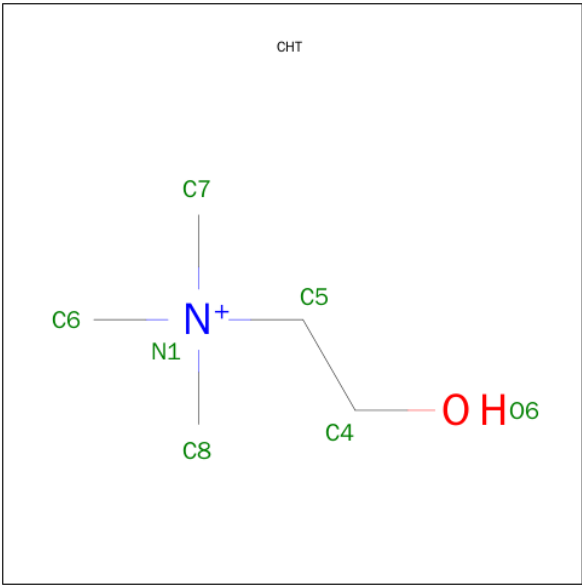
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C₄₀H₇₉O₁₀P).



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: C₅H₁₄NO).



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

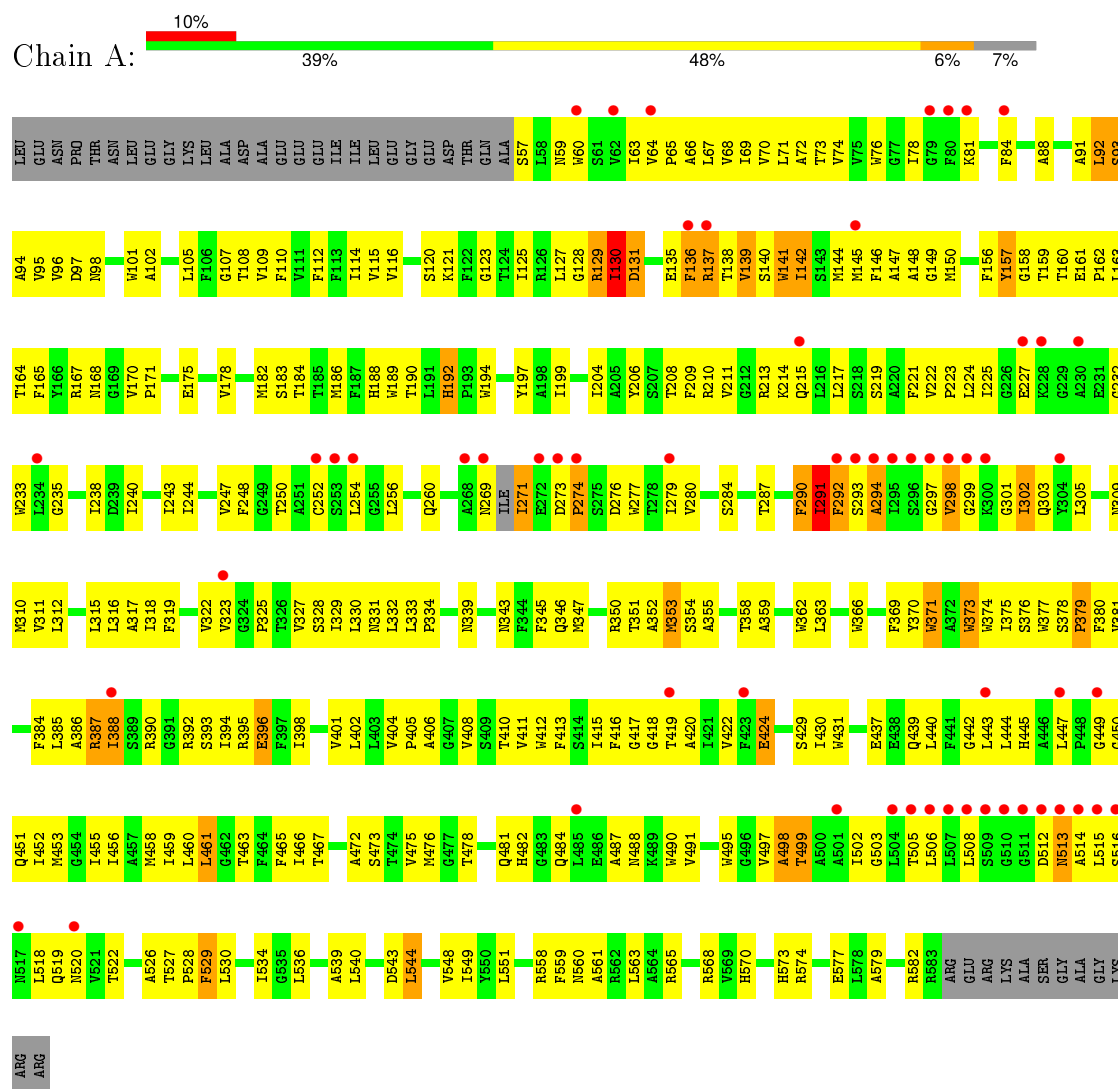
- Molecule 5 is water.

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

3 Residue-property plots

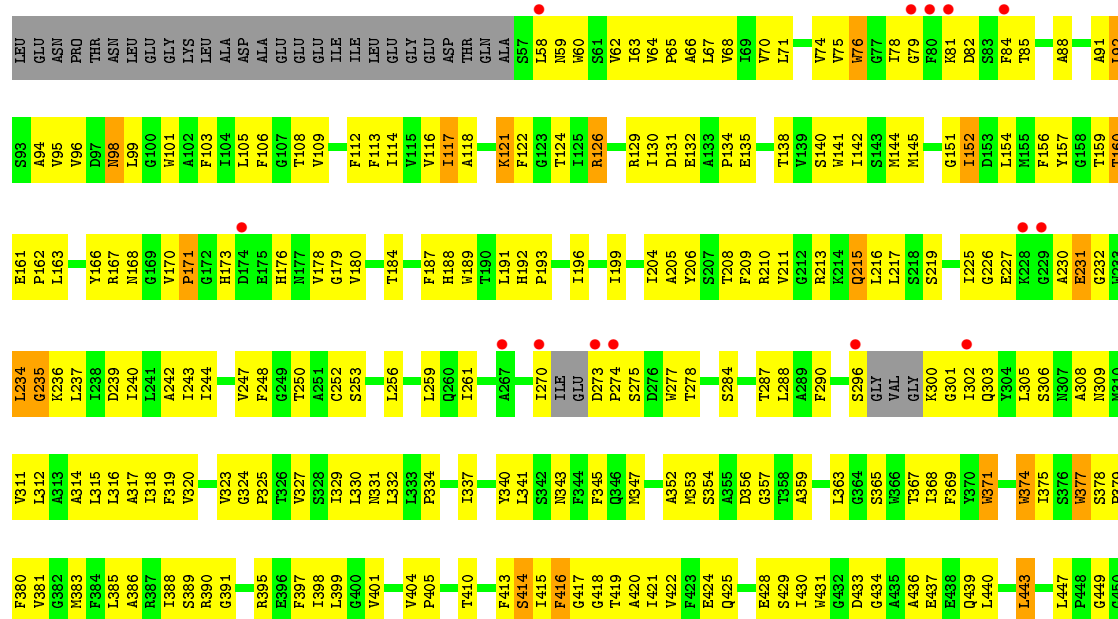
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Glycine betaine transporter BetP



• Molecule 1: Glycine betaine transporter BetP





GLY	Q451	Q451
ALA	I452	I452
GLY	M453	M453
LYS	G454	G454
ARG	I455	I455
ARG	I456	I456
	I459	I459
	L460	L460
	L461	L461
	G462	G462
	T463	T463
	F464	F464
	F465	F465
	I466	I466
	T467	T467
	S471	S471
	A472	A472
	S473	S473
	T474	T474
	V475	V475
	M476	M476
	M479	M479
	S480	S480
	Q481	Q481
	H482	H482
	G483	G483
	Q484	Q484
	L485	L485
	N488	N488
	V491	V491
	T492	T492
	A493	A493
	G496	G496
	I502	I502
	G503	G503
	L504	L504
	T505	T505
	L506	L506
	L507	L507
	L508	L508
	S509	S509
	N517	N517
	L518	L518
	Q519	Q519
	N520	N520
	V521	V521
	T522	T522
	I523	I523
	V524	V524
	T527	T527
	P528	P528

F529	F529
L530	L530
F531	F531
V532	V532
V533	V533
I534	I534
G535	G535
L536	L536
M537	M537
F538	F538
A539	A539
L540	L540
V541	V541
R542	R542
D543	D543
L544	L544
S545	S545
N546	N546
I549	I549
Y550	Y550
L551	L551
E552	E552
Y553	Y553
R554	R554
E555	E555
Q556	Q556
Q557	Q557
R558	R558
F559	F559
N560	N560
A561	A561
R562	R562
L563	L563
A564	A564
R565	R565
F566	F566
R567	R567
R568	R568
VAL	VAL
HIS	HIS
ASN	ASN
GLU	GLU
HIS	HIS
ARG	ARG
LYS	LYS
ARG	ARG
GLU	GLU
LEU	LEU
ALA	ALA
LYS	LYS
ARG	ARG
ARG	ARG
GLU	GLU
ARG	ARG
LYS	LYS
ALA	ALA
SER	SER

GLY	GLY
ALA	ALA
GLY	GLY
LYS	LYS
ARG	ARG
ARG	ARG

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	14.40 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.249 , 0.297 0.251 , 0.299	Depositor DCC
R_{free} test set	3842 reflections (11.03%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 38774 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGT, CHT, 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 [i](#)

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:B:154:LEU:HD12	1:B:154:LEU:O	1.73	0.87
1:A:302:ILE:HG22	1:A:303:GLN:H	1.38	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:C:284:SER:HA	1:C:287:THR:HG22	1.58	0.83
1:A:88:ALA:HB3	1:A:520:ASN:HD21	1.43	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:CD1	1:B:154:LEU:O	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:HD12	1:B:515:LEU:H	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:O	1:B:298:VAL:HG12	1.82	0.78
1:C:105:LEU:O	1:C:109:VAL:HG23	1.83	0.78
1:B:141:TRP:CH2	1:B:389:SER:HB3	2.18	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:CG	1:B:154:LEU:O	2.30	0.76
1:B:143:SER:HB2	1:B:306:SER:HB3	1.67	0.76
1:A:505:THR:HA	1:A:508:LEU:HG	1.68	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:C:163:LEU:HD22	1:C:420:ALA:HB1	1.68	0.75
1:A:64:VAL:HB	1:A:65:PRO:HD3	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:B:153:ASP:C	1:B:155:MET:H	1.90	0.72
1:A:209:PHE:CD2	1:A:390:ARG:HG2	2.24	0.72
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.71	0.72
1:B:259:LEU:HD13	1:B:437:GLU:HG2	1.72	0.72
1:B:515:LEU:CD1	1:B:515:LEU:H	2.02	0.72
1:B:134:PRO:O	1:B:135:GLU:HB2	1.87	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:B:473:SER:HA	1:B:476:MET:SD	2.31	0.70
1:A:373:TRP:C	1:A:373:TRP:CD1	2.62	0.70
1:A:260:GLN:HA	1:A:437:GLU:HG2	1.74	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:B:476:MET:HE2	1:B:495:TRP:HB3	1.77	0.67
1:A:375:ILE:HG22	1:A:529:PHE:HB3	1.77	0.67
1:B:515:LEU:N	1:B:515:LEU:HD12	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:B:384:PHE:CZ	1:B:471:SER:HB2	2.30	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:A:183:SER:OG	1:A:339:ASN:HB3	1.94	0.67
1:B:502:ILE:O	1:B:506:LEU:HG	1.94	0.67
1:B:92:LEU:O	1:B:95:VAL:HG12	1.95	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:C:456:ILE:O	1:C:459:ILE:HG22	1.94	0.66
1:B:265:LEU:HD22	1:B:269:ASN:HD21	1.60	0.66
1:C:485:LEU:HD12	1:C:485:LEU:H	1.60	0.66
1:A:211:VAL:HG11	1:A:213:ARG:HE	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:354:SER:O	1:C:359:ALA:HB3	1.96	0.66
1:C:122:PHE:CE1	1:C:544:LEU:HB3	2.30	0.66
1:A:312:LEU:HB3	1:A:460:LEU:HD21	1.77	0.66
1:A:515:LEU:N	1:A:515:LEU:HD12	2.10	0.66
1:A:170:VAL:HG13	1:A:171:PRO:HD2	1.76	0.66
1:B:152:ILE:CG1	1:B:464:PHE:HE1	2.09	0.66
1:A:141:TRP:O	1:A:145:MET:HG2	1.95	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:B:300:LYS:HG3	1:B:303:GLN:HB2	1.77	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:B:460:LEU:HA	1:B:463:THR:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD21	1:A:401:VAL:HG21	1.76	0.65
1:A:404:VAL:O	1:A:408:VAL:HG13	1.95	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:B:153:ASP:OD1	1:B:256:LEU:CG	2.45	0.65
1:A:252:CYS:HA	1:A:518:LEU:HD11	1.78	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:B:153:ASP:O	1:B:155:MET:N	2.29	0.64
1:A:373:TRP:C	1:A:373:TRP:HD1	2.01	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:H	1:B:217:LEU:HD12	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: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:121:LYS:HZ1	1:B:550:TYR:HD1	1.47	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:449:GLY:O	1:A:452:ILE:HG12	1.99	0.62
1:A:206:TYR:CE1	1:A:210:ARG:HG2	2.34	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:463:THR:O	1:A:467:THR:HG23	1.99	0.61
1:A:243:ILE:HD12	1:A:244:ILE:N	2.15	0.61
1:B:517:ASN:O	1:B:521:VAL:HG23	2.01	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:114:ILE:HB	1:A:398:ILE:HD13	1.82	0.61
1:C:121:LYS:N	1:C:121:LYS:HD3	2.15	0.61
1:B:234:LEU:H	1:B:234:LEU:HD12	1.65	0.61
1:A:69:ILE:HA	1:A:72:ALA:HB3	1.81	0.61
1:C:126:ARG:HD3	1:C:132:GLU:O	2.00	0.61
1:B:207:SER:O	1:B:213:ARG:HB2	2.01	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: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:66:ALA:O	1:A:70:VAL:HG23	2.01	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:C:230:ALA:O	1:C:231:GLU:HB3	2.01	0.60
1:A:456:ILE:HB	1:A:460:LEU:HD22	1.82	0.60
1:A:165:PHE:CE1	1:A:362:TRP:HZ2	2.20	0.60
1:A:92:LEU:HD12	1:A:93:SER:N	2.17	0.60
1:C:64:VAL:CG1	1:C:65:PRO:HD3	2.32	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:B:463:THR:C	1:B:465:PHE:H	2.06	0.59
1:A:142:ILE:H	1:A:142:ILE:HD13	1.66	0.59
1:B:157:TYR:HA	1:B:160:THR:HG22	1.82	0.59
1:C:122:PHE:CD1	1:C:544:LEU:HB3	2.37	0.59
1:A:81:LYS:CB	1:A:84:PHE:HB2	2.33	0.59
1:C:226:GLY:CA	1:C:227:GLU:HB3	2.20	0.59
1:A:527:THR:N	1:A:528:PRO:HD2	2.18	0.59
1:A:141:TRP:HH2	1:A:392:ARG:HG2	1.64	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:158:GLY:HA2	1:A:413:PHE:HE1	1.68	0.59
1:B:271:ILE:HG12	1:B:273:ASP:N	2.17	0.58
1:A:526:ALA:HB1	1:A:529:PHE:HB2	1.85	0.58
1:A:490:TRP:CD1	1:A:491:VAL:HG13	2.35	0.58
1:B:307:ASN:O	1:B:311:VAL:HG23	2.04	0.58
1:C:92:LEU:O	1:C:95:VAL:HG12	2.04	0.58
1:C:121:LYS:H	1:C:121:LYS:HD3	1.66	0.58
1:C:170:VAL:CG1	1:C:171:PRO:HD2	2.33	0.58
1:A:311:VAL:O	1:A:315:LEU:HB2	2.04	0.58
1:B:92:LEU:HD13	1:B:523:ILE:HG21	1.85	0.58
1:A:302:ILE:HG22	1:A:303:GLN:N	2.15	0.58
1:A:115:VAL:HG11	3:A:602:PGT:H402	1.85	0.58
1:A:579:ALA:O	1:A:582:ARG:HG2	2.03	0.58
1:A:123:GLY:O	1:A:395:ARG:HB2	2.02	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:CD	1:C:121:LYS:H	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: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: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: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:B:144:MET:SD	1:B:388:ILE:HD12	2.44	0.57
1:A:276:ASP:CG	1:A:277:TRP:H	2.08	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:378:SER:HA	1:A:381:VAL:HG22	1.85	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:A:442:GLY:HA2	1:A:445:HIS:CD2	2.39	0.57
1:A:112:PHE:CD1	3:A:602:PGT:H422	2.40	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: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:B:215:GLN:HE21	1:B:383:MET:HG3	1.69	0.57
1:A:387:ARG:NH1	1:A:387:ARG:HB3	2.19	0.56
1:C:227:GLU:H	1:C:230:ALA:CB	2.18	0.56
1:B:499:THR:O	1:B:502:ILE:HG12	2.05	0.56
1:C:309:ASN:HB3	1:C:464:PHE:CE1	2.40	0.56
1:B:190:THR:O	1:B:193:PRO:HD2	2.05	0.56
1:A:197:TYR:CE1	1:A:381:VAL:HG21	2.40	0.56
1:B:233:TRP:H	1:B:233:TRP:HD1	1.54	0.56
1:A:92:LEU:C	1:A:94:ALA:H	2.08	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:154:LEU:HD11	1:B:412:TRP:CD1	2.40	0.56
1:C:248:PHE:CD1	1:C:502:ILE:HD12	2.41	0.56
1:B:276:ASP:C	1:B:278:THR:H	2.09	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:C:64:VAL:HG13	1:C:65:PRO:HD3	1.86	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:B:476:MET:HE2	1:B:495:TRP:HE3	1.69	0.56
1:A:415:ILE:HG13	1:A:416:PHE:HD2	1.70	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:B:464:PHE:O	1:B:468:SER:OG	2.24	0.55
1:A:392:ARG:CD	1:A:396:GLU:HG3	2.35	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:B:118:ALA:HB2	1:B:398:ILE:HD12	1.88	0.55
1:A:558:ARG:O	1:A:561:ALA:HB3	2.05	0.55
1:A:331:ASN:ND2	1:B:352:ALA:HB3	2.22	0.55
1:C:475:VAL:O	1:C:479:MET:HG2	2.05	0.55
1:C:381:VAL:HG12	1:C:385:LEU:CD1	2.36	0.55
1:A:163:LEU:HD11	1:A:424:GLU:OE2	2.06	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: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:A:81:LYS:HB2	1:A:84:PHE:HB2	1.89	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:C:113:PHE:O	1:C:117:ILE:HG23	2.06	0.54
1:A:148:ALA:HB1	1:A:380:PHE:CZ	2.41	0.54
1:B:183:SER:OG	1:B:339:ASN:HB3	2.07	0.54
1:C:308:ALA:O	1:C:312:LEU:HD13	2.07	0.54
1:C:252:CYS:O	1:C:256:LEU:HG	2.08	0.54
1:C:126:ARG:HD2	1:C:131:ASP:HA	1.88	0.54
1:C:275:SER:HB3	1:C:278:THR:OG1	2.08	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:B:153:ASP:O	1:B:156:PHE:N	2.41	0.54
1:B:534:ILE:O	1:B:537:MET:HB3	2.08	0.54
1:B:134:PRO:O	1:B:135:GLU:CB	2.56	0.54
1:A:224:LEU:HD12	1:A:539:ALA:HB2	1.89	0.54
1:B:519:GLN:HE21	1:B:520:ASN:ND2	2.06	0.54
1:B:130:ILE:HD13	1:B:131:ASP:N	2.22	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:C:250:THR:HG22	1:C:377:TRP:HE1	1.73	0.54
1:A:366:TRP:O	1:A:369:PHE:HB3	2.07	0.54
1:B:451:GLN:H	1:B:451:GLN:CD	2.12	0.54
1:B:309:ASN:ND2	1:B:464:PHE:HB3	2.24	0.53
1:C:305:LEU:HA	1:C:308:ALA:HB3	1.89	0.53
1:A:527:THR:N	1:A:528:PRO:CD	2.71	0.53
1:B:108:THR:OG1	1:B:192:HIS:HE1	1.91	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:A:156:PHE:CE2	1:A:256:LEU:HD11	2.44	0.53
1:C:380:PHE:CE1	1:C:471:SER:HB2	2.43	0.53
1:A:235:GLY:H	1:A:238:ILE:HD13	1.73	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:114:ILE:HG23	1:B:199:ILE:HD12	1.88	0.53
1:B:435:ALA:O	1:B:438:GLU:HG2	2.08	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:B:150:MET:CE	1:B:154:LEU:HD23	2.37	0.53
1:C:488:ASN:HB3	1:C:491:VAL:HG12	1.90	0.53
1:B:384:PHE:CE1	1:B:471:SER:HB2	2.43	0.53
1:A:67:LEU:HA	1:A:70:VAL:HB	1.91	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:B:153:ASP:C	1:B:155:MET:N	2.58	0.53
1:A:498:ALA:O	1:A:499:THR:HB	2.09	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:C:421:ILE:O	1:C:425:GLN:HG3	2.09	0.53
1:B:111:VAL:HG22	1:B:191:LEU:O	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:C:226:GLY:CA	1:C:227:GLU:CB	2.83	0.52
1:A:88:ALA:CB	1:A:520:ASN:HD21	2.17	0.52
1:C:517:ASN:O	1:C:521:VAL:HG22	2.09	0.52
1:B:305:LEU:HB3	1:B:467:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:N	1:A:223:PRO:CD	2.72	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:C:230:ALA:O	1:C:231:GLU:CB	2.56	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: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: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:187:PHE:CD1	1:B:347:MET:HG3	2.45	0.52
1:B:371:TRP:CE3	1:B:374:TRP:HD1	2.27	0.52
1:B:298:VAL:CG1	1:B:298:VAL:O	2.54	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:512:ASP:O	1:B:513:ASN:HB2	2.08	0.51
1:B:249:GLY:O	1:B:253:SER:OG	2.28	0.51
1:B:204:ILE:HD11	1:B:217:LEU:HA	1.93	0.51
1:C:94:ALA:O	1:C:98:ASN:OD1	2.28	0.51
1:A:101:TRP:CE2	1:C:330:LEU:HD13	2.44	0.51
1:B:279:ILE:O	1:B:283:VAL:HB	2.10	0.51
1:B:76:TRP:O	1:B:85:THR:HB	2.09	0.51
1:A:515:LEU:CD1	1:A:515:LEU:N	2.73	0.51
1:A:254:LEU:HD22	1:A:465:PHE:CZ	2.45	0.51
1:B:260:GLN:HG2	1:B:461:LEU:HD22	1.93	0.51
1:A:74:VAL:HG13	1:A:502:ILE:HB	1.93	0.51
1:A:506:LEU:C	1:A:506:LEU:CD2	2.76	0.51
1:A:318:ILE:O	1:A:322:VAL:HG22	2.10	0.51
1:A:149:GLY:HA2	1:A:381:VAL:CG1	2.41	0.51
1:C:67:LEU:HA	1:C:70:VAL:CG1	2.38	0.51
1:A:156:PHE:CD2	1:A:256:LEU:HD11	2.46	0.51
1:B:103:PHE:HE1	1:B:372:ALA:HA	1.75	0.51
1:A:352:ALA:HB3	1:C:331:ASN:ND2	2.26	0.51
1:B:364:GLY:HA2	1:B:368:ILE:HB	1.91	0.51
1:B:128:GLY:HA2	1:B:209:PHE:O	2.10	0.51
1:A:112:PHE:HZ	1:A:345:PHE:CZ	2.29	0.51
1:C:225:ILE:HG22	1:C:226:GLY:O	2.10	0.51
1:A:393:SER:HB3	1:A:396:GLU:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:HH11	1:C:552:GLU:HG3	1.74	0.51
1:C:404:VAL:CB	1:C:405:PRO:HD3	2.39	0.51
1:A:160:THR:O	1:A:164:THR:HG22	2.11	0.51
1:B:374:TRP:HA	1:B:374:TRP:CE3	2.46	0.51
1:A:74:VAL:O	1:A:78:ILE:HG22	2.11	0.51
1:C:551:LEU:O	1:C:555:GLU:HG3	2.10	0.51
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:186:MET:HE3	1:A:190:THR:HG21	1.92	0.50
1:B:196:ILE:HD11	1:B:374:TRP:CB	2.27	0.50
1:C:524:VAL:O	1:C:528:PRO:HD3	2.11	0.50
1:A:121:LYS:CG	3:A:602:PGT:H11	2.41	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:A:142:ILE:CD1	1:A:142:ILE:H	2.23	0.50
1:B:375:ILE:HG12	1:B:530:LEU:HA	1.92	0.50
1:A:292:PHE:HA	1:A:293:SER:O	2.11	0.50
1:A:136:PHE:O	1:A:137:ARG:CB	2.59	0.50
1:B:70:VAL:O	1:B:74:VAL:HG12	2.11	0.50
1:A:63:ILE:O	1:A:66:ALA:HB3	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:B:232:GLY:O	1:B:233:TRP:C	2.49	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:C:129:ARG:NH1	1:C:130:ILE:H	2.09	0.50
1:B:206:TYR:O	1:B:210:ARG:HB3	2.11	0.50
1:B:176:HIS:N	1:B:176:HIS:CD2	2.79	0.50
1:A:273:ASP:HB3	1:A:274:PRO:CD	2.39	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:81:LYS:HB3	1:A:84:PHE:HB2	1.94	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:B:458:MET:HA	1:B:461:LEU:CD1	2.36	0.49
1:A:451:GLN:O	1:A:455:ILE:HG13	2.10	0.49
1:B:250:THR:O	1:B:254:LEU:HG	2.12	0.49
1:B:455:ILE:HG13	1:B:456:ILE:N	2.26	0.49
1:A:330:LEU:HG	1:B:101:TRP:CG	2.47	0.49
1:A:161:GLU:HB3	1:A:162:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:SER:O	1:B:359:ALA:HB3	2.12	0.49
1:B:540:LEU:O	1:B:544:LEU:HG	2.11	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: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:C:284:SER:HA	1:C:287:THR:CG2	2.36	0.49
1:C:66:ALA:N	1:C:240:ILE:HD11	2.27	0.49
1:B:129:ARG:O	1:B:130:ILE:HG22	2.13	0.49
1:C:520:ASN:O	1:C:524:VAL:HG23	2.12	0.49
3:A:602:PGT:H12	3:A:602:PGT:O31	2.11	0.49
1:A:455:ILE:HG23	1:A:459:ILE:HD12	1.95	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:A:156:PHE:HE1	1:A:437:GLU:HG3	1.78	0.49
1:B:234:LEU:N	1:B:234:LEU:HD12	2.28	0.49
1:B:305:LEU:HB3	1:B:467:THR:CG2	2.43	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:A:159:THR:OG1	1:A:443:LEU:HD21	2.12	0.49
1:C:449:GLY:O	1:C:452:ILE:HG12	2.13	0.49
1:A:430:ILE:HG13	1:A:443:LEU:HB3	1.95	0.49
1:B:399:LEU:C	1:B:399:LEU:HD12	2.33	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:430:ILE:HG21	1:C:443:LEU:HA	1.96	0.48
1:C:76:TRP:C	1:C:76:TRP:CD1	2.86	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:B:186:MET:HE1	1:B:336:SER:HB3	1.95	0.48
1:A:370:TYR:C	1:A:374:TRP:CD1	2.87	0.48
1:B:141:TRP:HD1	1:B:145:MET:SD	2.36	0.48
1:A:497:VAL:O	1:A:499:THR:N	2.45	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:380:PHE:CD1	1:A:472:ALA:HA	2.48	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: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:A:128:GLY:O	1:A:129:ARG:C	2.51	0.48
1:B:467:THR:HA	1:B:470:ASP:OD2	2.14	0.48
1:B:316:LEU:O	1:B:319:PHE:HB3	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:473:SER:HA	1:A:476:MET:HG2	1.96	0.48
1:A:95:VAL:HG23	1:A:96:VAL:N	2.29	0.48
1:B:476:MET:HA	1:B:479:MET:HG2	1.96	0.47
1:A:162:PRO:HG2	1:A:417:GLY:HA3	1.96	0.47
1:B:519:GLN:HA	5:B:608:HOH:O	2.14	0.47
1:B:194:TRP:CE3	1:B:197:TYR:HD2	2.32	0.47
1:B:325:PRO:HB2	1:B:328:SER:HB2	1.95	0.47
1:B:254:LEU:HA	1:B:465:PHE:CZ	2.49	0.47
1:A:188:HIS:HA	1:A:371:TRP:HH2	1.79	0.47
1:A:94:ALA:O	1:A:98:ASN:HB2	2.14	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:B:371:TRP:HE3	1:B:374:TRP:HD1	1.61	0.47
1:B:100:GLY:O	1:B:104:ILE:HG13	2.15	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:B:443:LEU:HD12	1:B:443:LEU:O	2.14	0.47
1:A:418:GLY:O	1:A:422:VAL:HG23	2.14	0.47
1:B:280:VAL:O	1:B:284:SER:HB3	2.15	0.47
1:A:222:VAL:CG2	1:A:223:PRO:HD3	2.44	0.47
1:B:486:GLU:H	1:B:486:GLU:CD	2.18	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:A:194:TRP:CE3	1:A:197:TYR:HD2	2.33	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: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:A:67:LEU:HD12	1:A:67:LEU:H	1.80	0.47
1:B:276:ASP:O	1:B:278:THR:N	2.44	0.47
1:A:250:THR:O	1:A:254:LEU:HG	2.15	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: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:B:136:PHE:HB3	1:B:140:SER:HB2	1.97	0.46
1:A:297:GLY:CA	1:A:298:VAL:HG22	2.46	0.46
1:A:167:ARG:HG2	1:A:168:ASN:OD1	2.15	0.46
1:C:415:ILE:O	1:C:419:THR:HG23	2.15	0.46
1:B:112:PHE:O	1:B:116:VAL:HG23	2.15	0.46
1:C:451:GLN:O	1:C:455:ILE:HG13	2.16	0.46
1:A:370:TYR:O	1:A:374:TRP:CD1	2.68	0.46
1:A:247:VAL:HG13	1:A:498:ALA:HB1	1.98	0.46
1:A:208:THR:HG21	1:A:215:GLN:CD	2.35	0.46
1:C:141:TRP:HD1	1:C:388:ILE:HG22	1.81	0.46
1:B:151:GLY:O	1:B:155:MET:HG3	2.15	0.46
1:C:377:TRP:C	1:C:379:PRO:HD2	2.35	0.46
1:A:574:ARG:HA	1:A:577:GLU:HG2	1.98	0.46
1:B:430:ILE:O	1:B:430:ILE:HD12	2.16	0.46
1:A:88:ALA:HA	1:A:91:ALA:HB3	1.98	0.46
1:C:151:GLY:O	1:C:152:ILE:C	2.54	0.46
1:A:125:ILE:O	1:A:394:ILE:HG12	2.16	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: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:B:322:VAL:HG23	1:B:323:VAL:N	2.30	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:150:MET:HE2	1:B:154:LEU:CD2	2.41	0.46
1:A:243:ILE:O	1:A:247:VAL:HG23	2.15	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:B:344:PHE:O	1:B:348:ALA:HB2	2.16	0.46
1:A:346:GLN:HG2	1:A:346:GLN:O	2.16	0.46
1:A:188:HIS:HA	1:A:371:TRP:CH2	2.51	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:250:THR:HG21	1:C:472:ALA:HB1	1.97	0.45
1:A:512:ASP:O	1:A:513:ASN:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:HH22	1:C:549:ILE:CG1	2.29	0.45
1:B:139:VAL:HG12	1:B:139:VAL: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:B:71:LEU:HD23	1:B:71:LEU:O	2.16	0.45
1:A:178:VAL:O	1:A:182:MET:HG2	2.16	0.45
1:A:332:LEU:HD23	1:A:332:LEU:O	2.17	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:302:ILE:HG23	1:A:305:LEU:HD21	1.99	0.45
1:A:105:LEU:O	1:A:109:VAL:HG23	2.17	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:A:108:THR:HA	1:A:192:HIS:NE2	2.32	0.45
1:C:225:ILE:CG2	1:C:226:GLY:N	2.79	0.45
1:C:428:GLU:N	1:C:428:GLU:OE1	2.49	0.45
1:A:393:SER:HB3	1:A:396:GLU:HG2	1.98	0.45
1:A:301:GLY:CA	1:A:302:ILE:C	2.85	0.45
1:B:141:TRP:CZ2	1:B:389:SER:HB3	2.50	0.45
1:A:333:LEU:HB3	1:A:334:PRO:HD3	1.99	0.45
1:A:269:ASN:O	1:A:271:ILE:HB	2.16	0.45
1:B:547:ASP:OD1	1:B:548:VAL:HG22	2.16	0.45
1:B:374:TRP:HA	1:B:374:TRP:HE3	1.81	0.45
1:C:417:GLY:O	1:C:421:ILE:HG12	2.17	0.45
1:B:300:LYS:CG	1:B:303:GLN:HB2	2.45	0.45
1:C:60:TRP:C	1:C:62:VAL:H	2.20	0.45
1:A:558:ARG:HA	1:A:558:ARG:HH11	1.82	0.45
1:A:159:THR:HG21	1:A:440:LEU:HA	1.99	0.45
1:B:161:GLU:HG2	1:B:185:THR:OG1	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:A:343:ASN:O	1:A:347:MET:HG3	2.16	0.44
1:B:373:TRP:C	1:B:373:TRP:CD1	2.88	0.44
1:C:91:ALA:O	1:C:94:ALA:HB3	2.17	0.44
1:A:57:SER:HB2	1:A:482:HIS:ND1	2.32	0.44
1:A:107:GLY:O	1:A:110:PHE:HB2	2.17	0.44
1:C:375:ILE:CD1	1:C:530:LEU:HD13	2.47	0.44
1:A:139:VAL:HG23	1:A:140:SER:H	1.82	0.44
1:B:193:PRO:HG3	1:B:374:TRP:NE1	2.31	0.44
1:C:208:THR:HG21	1:C:215:GLN:CG	2.46	0.44
1:B:505:THR:HA	1:B:508:LEU:HG	1.99	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:B:189:TRP:CZ2	1:B:370:TYR:OH	2.69	0.44
1:B:371:TRP:HA	1:B:371:TRP:CE3	2.52	0.44
1:B:371:TRP:HA	1:B:371:TRP:HE3	1.82	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:C:82:ASP:O	1:C:85:THR:HG22	2.16	0.44
1:B:240:ILE:O	1:B:244:ILE:HG13	2.16	0.44
1:C:259:LEU:HD13	1:C:437:GLU:OE1	2.18	0.44
1:C:527:THR:N	1:C:528:PRO:CD	2.81	0.44
1:C:476:MET:HA	1:C:479:MET:HE2	2.00	0.44
1:A:101:TRP:CG	1:A:102:ALA:N	2.85	0.44
1:C:225:ILE:O	1:C:227:GLU:HB2	2.18	0.44
1:B:151:GLY:O	1:B:155:MET:CG	2.66	0.44
1:A:514:ALA:C	1:A:515:LEU:HD12	2.37	0.44
1:C:74:VAL:HG12	1:C:505:THR:OG1	2.18	0.44
1:A:333:LEU:HB3	1:A:334:PRO:CD	2.47	0.44
1:C:159:THR:CG2	1:C:416:PHE:HB3	2.48	0.44
1:A:223:PRO:HG2	1:A:543:ASP:HB2	1.99	0.44
1:A:146:PHE:O	1:A:147:ALA:C	2.56	0.44
1:A:381:VAL:O	1:A:385:LEU:HB2	2.17	0.44
1:C:206:TYR:CE2	1:C:211:VAL:HG23	2.53	0.44
1:C:62:VAL:C	1:C:65:PRO:HD2	2.38	0.44
1:C:187:PHE:HA	1:C:340:TYR:HE1	1.83	0.44
1:A:167:ARG:NH1	1:A:431:TRP:CG	2.85	0.44
1:C:99:LEU:HD11	1:C:531:PHE:HZ	1.82	0.44
1:B:106:PHE:HB3	1:B:110:PHE:CZ	2.53	0.44
1:A:92:LEU:C	1:A:92:LEU:HD12	2.39	0.44
1:A:204:ILE:HD11	1:A:217:LEU:HD12	2.00	0.44
1:C:141:TRP:CD1	1:C:388:ILE:HG22	2.53	0.44
1:C:371:TRP:CE3	1:C:371:TRP:HA	2.53	0.44
1:C:114:ILE:HA	1:C:114:ILE:HD12	1.81	0.43
1:B:276:ASP:O	1:B:277:TRP:CD1	2.71	0.43
1:B:186:MET:CE	1:B:336:SER:HB3	2.48	0.43
1:A:540:LEU:HD22	1:A:544:LEU:HD22	2.00	0.43
1:B:149:GLY:O	1:B:150:MET:HG3	2.18	0.43
1:B:141:TRP:O	1:B:142:ILE:C	2.56	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: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
1:C:193:PRO:O	1:C:196:ILE:HB	2.18	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:A:497:VAL:O	1:A:498:ALA:C	2.56	0.43
1:A:199:ILE:HG22	1:A:536:LEU:HD23	2.00	0.43
1:C:173:HIS:CD2	1:C:180:VAL:HG11	2.53	0.43
1:B:256:LEU:O	1:B:256:LEU:HD13	2.18	0.43
1:A:189:TRP:CZ3	1:A:374:TRP:HH2	2.37	0.43
1:B:64:VAL:O	1:B:68:VAL:HG22	2.18	0.43
1:A:481:GLN:O	1:A:484:GLN:HG2	2.18	0.43
1:C:371:TRP:CE3	1:C:371:TRP:CA	3.02	0.43
1:A:536:LEU:O	1:A:540:LEU:HB2	2.18	0.43
1:C:124:THR:HG23	1:C:395:ARG:HH21	1.83	0.43
1:B:271:ILE:HG12	1:B:272:GLU:CA	2.49	0.43
1:A:115:VAL:CG1	3:A:602:PGT:H402	2.48	0.43
1:B:233:TRP:HB2	1:B:234:LEU:HD12	2.00	0.43
1:B:157:TYR:HD1	1:B:160:THR:CG2	2.31	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: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: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:156:PHE:O	1:A:156:PHE:CG	2.71	0.43
1:B:74:VAL:CG2	1:B:502:ILE:HB	2.49	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:473:SER:HA	1:A:476:MET:SD	2.59	0.43
1:C:216:LEU:HD21	1:C:483:GLY:N	2.34	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:C:103:PHE:HZ	1:C:527:THR:HG22	1.84	0.43
1:A:445:HIS:HA	1:A:450:GLY:CA	2.38	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:505:THR:HA	1:A:508:LEU:CG	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:VAL:HG23	1:C:522:THR:N	2.33	0.42
1:A:92:LEU:C	1:A:94:ALA:N	2.73	0.42
1:C:546:ASN:O	1:C:551:LEU:HD12	2.19	0.42
1:A:190:THR:HB	1:A:406:ALA:HB1	2.00	0.42
1:B:127:LEU:O	1:B:127:LEU:HG	2.19	0.42
1:A:563:LEU:C	1:A:563:LEU:HD23	2.39	0.42
1:A:232:GLY:O	1:A:233:TRP:C	2.56	0.42
1:B:254:LEU:CD2	1:B:465:PHE:CE1	2.85	0.42
1:B:141:TRP:HH2	1:B:389:SER:CB	2.30	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:C:316:LEU:HB3	1:C:416:PHE:HZ	1.84	0.42
1:A:443:LEU:C	1:A:443:LEU:HD12	2.38	0.42
1:B:463:THR:C	1:B:465:PHE:N	2.71	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:B:141:TRP:O	1:B:143:SER:N	2.52	0.42
1:A:502:ILE:HA	1:A:505:THR:OG1	2.18	0.42
1:C:60:TRP:O	1:C:64:VAL:HG12	2.19	0.42
1:A:182:MET:CE	1:A:332:LEU:HD21	2.49	0.42
1:A:559:PHE:O	1:A:560:ASN:C	2.57	0.42
1:A:290:PHE:CE2	1:A:291:ILE:HG23	2.54	0.42
1:B:189:TRP:HZ2	1:B:370:TYR:OH	2.02	0.42
1:A:371:TRP:CE3	1:A:371:TRP:HA	2.54	0.42
1:C:337:ILE:O	1:C:341:LEU:HG	2.20	0.42
1:C:303:GLN:HA	1:C:306:SER:HB3	2.01	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:C:475:VAL:HG12	1:C:479:MET:CE	2.49	0.42
1:B:331:ASN:HD22	1:C:352:ALA:HB3	1.84	0.42
1:C:330:LEU:HD23	1:C:330:LEU:HA	1.89	0.42
1:B:158:GLY:HA2	1:B:413:PHE:CE1	2.54	0.42
1:C:154:LEU:HD23	1:C:413:PHE:CE2	2.54	0.42
1:C:353:MET:O	1:C:357:GLY:N	2.49	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:C:78:ILE:CG2	1:C:505:THR:HG23	2.41	0.42
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: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:B:199:ILE:HG22	1:B:200:VAL:N	2.34	0.42
1:A:208:THR:HG21	1:A:215:GLN:HA	2.01	0.42
1:B:286:LEU:HD23	1:B:465:PHE:CD2	2.55	0.42
1:A:66:ALA:HB1	1:A:243:ILE:HD13	2.01	0.42
1:C:145:MET:CE	1:C:404:VAL:HG21	2.50	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:527:THR:OG1	1:C:528:PRO:HD3	2.20	0.42
1:C:166:TYR:CE2	1:C:176:HIS:HD2	2.38	0.42
1:C:81:LYS:HB3	1:C:84:PHE:HD2	1.80	0.42
1:B:233:TRP:N	1:B:233:TRP:CD1	2.84	0.42
1:B:222:VAL:HB	1:B:223:PRO:HD3	2.00	0.42
1:A:279:ILE:HG22	1:A:279:ILE:O	2.19	0.42
1:B:152:ILE:HA	1:B:464:PHE:CZ	2.55	0.42
1:A:67:LEU:HD11	1:A:495:TRP:CH2	2.55	0.42
1:B:104:ILE:HD12	1:B:105:LEU:N	2.35	0.42
1:C:377:TRP:CH2	4:C:601:CHT:HC51	2.54	0.42
1:B:234:LEU:H	1:B:234:LEU:CD1	2.32	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: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:B:264:GLY:HA3	1:B:458:MET:SD	2.60	0.42
1:A:305:LEU:HD22	1:A:467:THR:HA	2.02	0.42
1:C:284:SER:CA	1:C:287:THR:HG22	2.41	0.42
1:A:243:ILE:HD12	1:A:244:ILE:HG13	2.01	0.42
1:B:68:VAL:HG23	1:B:69:ILE:N	2.35	0.42
1:B:319:PHE:O	1:B:323:VAL:HG22	2.20	0.42
1:A:456:ILE:HB	1:A:460:LEU:CD1	2.49	0.41
1:B:213:ARG:HH11	1:B:222:VAL:HB	1.85	0.41
1:A:568:ARG:HH11	1:C:552:GLU:CG	2.33	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:371:TRP:CA	1:A:371:TRP:CE3	3.03	0.41
1:A:78:ILE:HD13	1:A:505:THR:O	2.21	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
1:A:204:ILE:O	1:A:208:THR:HG23	2.19	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.82	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:HD12	1:A:105:LEU:O	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:384:PHE:HA	1:A:387:ARG:HD2	2.02	0.41
1:A:170:VAL:CG1	1:A:171:PRO:HD2	2.49	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:B:144:MET:SD	1:B:384:PHE:HD2	2.44	0.41
1:B:473:SER:O	1:B:476:MET:HB2	2.21	0.41
1:B:371:TRP:CE3	1:B:374:TRP:CD1	3.08	0.41
1:A:136:PHE:HD1	1:A:388:ILE:HB	1.85	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:A:116:VAL:O	1:A:120:SER:N	2.52	0.41
1:C:323:VAL:HG13	1:C:324:GLY:N	2.35	0.41
1:A:219:SER:O	1:A:222:VAL:HG13	2.20	0.41
1:A:114:ILE:CD1	1:A:402:LEU:HD11	2.51	0.41
1:B:214:LYS:HB3	1:B:214:LYS:HE2	1.87	0.41
1:A:189:TRP:CZ2	1:A:370:TYR:HE1	2.38	0.41
1:A:354:SER:HA	1:A:355:ALA:HA	1.71	0.41
1:C:210:ARG:NH2	1:C:549:ILE:HG12	2.35	0.41
1:A:158:GLY:HA2	1:A:413:PHE:CE1	2.53	0.41
1:A:484:GLN:H	1:A:484:GLN:HG2	1.70	0.41
1:C:88:ALA:O	1:C:91:ALA:HB3	2.21	0.41
1:C:325:PRO:HD2	1:C:419:THR:HG22	2.02	0.41
1:B:432:GLY:C	1:B:434:GLY:H	2.23	0.41
1:A:299:GLY:HA2	1:A:487:ALA:HB2	2.03	0.41
1:C:466:ILE:HD12	1:C:466:ILE:N	2.35	0.41
1:A:110:PHE:CZ	1:A:534:ILE:HD13	2.56	0.41
1:A:65:PRO:C	1:A:68:VAL:HG12	2.41	0.41
1:C:159:THR:HA	1:C:417:GLY:CA	2.50	0.41
1:C:323:VAL:HG13	1:C:447:LEU:HD13	2.02	0.41
1:A:170:VAL:HG22	1:A:362:TRP:CZ2	2.55	0.41
1:C:290:PHE:CE2	1:C:496:GLY:HA3	2.56	0.41
1:C:124:THR:HG23	1:C:395:ARG:NH2	2.35	0.41
1:A:280:VAL:O	1:A:284:SER:HB2	2.20	0.41
1:A:130:ILE:HB	1:A:131:ASP:H	1.65	0.41
1:A:327:VAL:HG21	1:B:98:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LEU:CA	1:B:463:THR:HG22	2.48	0.41
1:B:476:MET:HE2	1:B:495:TRP:CE3	2.52	0.41
1:A:145:MET:CE	1:A:385:LEU:HD13	2.51	0.41
1:B:150:MET:HE3	1:B:154:LEU:CD2	2.48	0.41
1:A:415:ILE:O	1:A:419:THR:HG23	2.21	0.41
1:A:60:TRP:HA	1:A:63:ILE:HG22	2.03	0.41
1:B:466:ILE:O	1:B:470:ASP:HB3	2.21	0.41
1:A:81:LYS:HB2	1:A:84:PHE:CB	2.50	0.41
1:C:129:ARG:HH12	1:C:130:ILE:HG13	1.85	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:C:556:GLN:O	1:C:560:ASN:HB2	2.20	0.41
1:A:410:THR:HG23	1:A:411:VAL:N	2.35	0.41
1:B:444:LEU:HA	1:B:444:LEU:HD23	1.87	0.41
1:C:270:ILE:HD12	1:C:270:ILE:N	2.36	0.41
1:B:455:ILE:CG1	1:B:456:ILE:N	2.83	0.41
1:A:156:PHE:O	1:A:156:PHE:CD2	2.74	0.41
1:C:440:LEU:O	1:C:443:LEU:HB3	2.21	0.41
1:B:372:ALA:HB1	1:B:523:ILE:HG23	2.03	0.41
1:A:163:LEU:HD22	1:A:420:ALA:HB1	2.02	0.41
1:A:175:GLU:HG2	1:A:175:GLU:H	1.74	0.41
1:B:453:MET:O	1:B:456:ILE:HG12	2.21	0.40
1:A:329:ILE:HD13	1:A:415:ILE:HG22	2.02	0.40
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:B:320:VAL:HG12	1:B:447:LEU:HD13	2.03	0.40
1:A:424:GLU:N	1:A:424:GLU:OE1	2.54	0.40
1:C:329:ILE:HD11	1:C:419:THR:CG2	2.51	0.40
1:A:516:SER:C	1:A:518:LEU:H	2.24	0.40
1:A:209:PHE:HE2	1:A:386:ALA:O	2.03	0.40
1:C:453:MET:HA	1:C:456:ILE:HD12	2.03	0.40
1:B:320:VAL:HG12	1:B:447:LEU:CD1	2.51	0.40
1:B:175:GLU:CD	1:B:175:GLU:H	2.25	0.40
1:B:475:VAL:HG22	1:B:479:MET:HE2	2.04	0.40
1:A:301:GLY:HA2	1:A:302:ILE:CB	2.41	0.40
1:B:207:SER:HA	1:B:213:ARG:HH21	1.86	0.40
1:C:64:VAL:N	1:C:65:PRO:CD	2.85	0.40
1:B:58:LEU:CD2	1:B:481:GLN:HE21	2.35	0.40
1:C:371:TRP:HE3	1:C:371:TRP:N	2.20	0.40
1:B:81:LYS:NZ	1:B:84:PHE:HD2	2.20	0.40
1:B:147:ALA:O	1:B:468:SER:OG	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:O	1:A:450:GLY:HA2	2.21	0.40
1:A:316:LEU:HD11	1:A:412:TRP:HH2	1.87	0.40
1:B:466:ILE:O	1:B:466:ILE:HD12	2.22	0.40
1:C:213:ARG:HD2	1:C:219:SER:O	2.20	0.40
1:A:184:THR:N	1:A:347:MET:HE1	2.37	0.40
1:A:213:ARG:HB2	1:A:214:LYS:H	1.72	0.40
1:C:536:LEU:O	1:C:540:LEU:HB2	2.22	0.40
1:B:330:LEU:HG	1:C:101:TRP:CE2	2.57	0.40
1:C:389:SER:O	1:C:390:ARG:C	2.58	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:B:122:PHE:CD1	1:B:544:LEU:HB3	2.57	0.40
1:C:184:THR:HG22	1:C:188:HIS:CE1	2.57	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%)	4	28
1	B	497/566 (88%)	406 (82%)	76 (15%)	15 (3%)	5	35
1	C	501/566 (88%)	411 (82%)	81 (16%)	9 (2%)	11	49
All	All	1522/1698 (90%)	1231 (81%)	247 (16%)	44 (3%)	6	36

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 ⓘ

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%)	29	69
1	B	391/443 (88%)	351 (90%)	40 (10%)	9	35
1	C	397/443 (90%)	370 (93%)	27 (7%)	20	58
All	All	1200/1329 (90%)	1112 (93%)	88 (7%)	17	55

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

Some 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.81	2 (4%)	51,56,56	1.11	3 (5%)
4	CHT	C	601	-	6,6,6	0.82	0	8,8,8	0.37	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	-	-	0/55/55/55	0/0/0/0
4	CHT	C	601	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	PGT	O2-C2	-2.79	1.39	1.46
3	A	602	PGT	O3-C3	-2.38	1.39	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	PGT	O3-C11-C12	2.32	118.97	111.90
3	A	602	PGT	O3-C3-C2	3.14	117.14	108.69
3	A	602	PGT	O2-C31-C32	4.27	120.81	111.53

There are no chirality outliers.

There are no torsion outliers.

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

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, 95th 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%)	0.50	58 (11%) 7 5	22, 120, 299, 416	0
1	B	501/566 (88%)	0.40	65 (12%) 5 3	13, 116, 284, 438	0
1	C	507/566 (89%)	-0.14	22 (4%) 39 29	9, 75, 181, 389	0
All	All	1534/1698 (90%)	0.25	145 (9%) 10 8	9, 98, 275, 438	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	ILE	20.7
1	A	299	GLY	17.3
1	C	81	LYS	13.2
1	A	513	ASN	11.0
1	A	294	ALA	9.6
1	B	512	ASP	8.2
1	B	505	THR	7.5
1	A	505	THR	7.4
1	B	508	LEU	7.2
1	A	509	SER	7.1
1	B	550	TYR	7.0
1	A	296	SER	6.9
1	A	298	VAL	6.8
1	B	234	LEU	6.8
1	A	227	GLU	6.1
1	B	504	LEU	6.1
1	A	516	SER	6.0
1	A	304	TYR	6.0
1	A	506	LEU	5.9
1	B	273	ASP	5.8
1	B	79	GLY	5.7
1	B	125	ILE	5.6
1	C	273	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	568	ARG	5.0
1	C	84	PHE	5.0
1	C	555	GLU	4.9
1	B	509	SER	4.9
1	A	517	ASN	4.8
1	B	551	LEU	4.6
1	A	512	ASP	4.5
1	A	508	LEU	4.5
1	A	274	PRO	4.4
1	C	274	PRO	4.4
1	C	270	ILE	4.3
1	B	225	ILE	4.2
1	A	80	PHE	4.0
1	A	501	ALA	4.0
1	A	137	ARG	3.9
1	A	268	ALA	3.9
1	A	504	LEU	3.9
1	A	292	PHE	3.8
1	B	80	PHE	3.8
1	B	297	GLY	3.7
1	A	273	ASP	3.7
1	A	300	LYS	3.7
1	B	391	GLY	3.6
1	B	275	SER	3.6
1	C	562	ARG	3.6
1	A	234	LEU	3.6
1	B	85	THR	3.6
1	A	136	PHE	3.5
1	B	252	CYS	3.5
1	B	390	ARG	3.5
1	B	127	LEU	3.5
1	A	252	CYS	3.5
1	B	251	ALA	3.4
1	B	556	GLN	3.4
1	C	79	GLY	3.4
1	A	81	LYS	3.4
1	A	254	LEU	3.4
1	A	269	ASN	3.4
1	C	296	SER	3.3
1	B	490	TRP	3.3
1	B	76	TRP	3.3
1	B	274	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	513	ASN	3.2
1	B	272	GLU	3.1
1	B	129	ARG	3.1
1	A	228	LYS	3.1
1	B	151	GLY	3.1
1	B	510	GLY	3.1
1	B	141	TRP	3.1
1	B	295	ILE	3.1
1	A	279	ILE	3.0
1	B	253	SER	3.0
1	A	447	LEU	3.0
1	A	64	VAL	3.0
1	C	174	ASP	2.9
1	A	60	TRP	2.9
1	B	393	SER	2.9
1	B	501	ALA	2.9
1	B	271	ILE	2.8
1	B	396	GLU	2.8
1	B	552	GLU	2.8
1	C	80	PHE	2.8
1	C	228	LYS	2.8
1	B	517	ASN	2.8
1	B	511	GLY	2.7
1	C	302	ILE	2.7
1	C	267	ALA	2.7
1	B	84	PHE	2.7
1	B	224	LEU	2.7
1	A	443	LEU	2.7
1	B	265	LEU	2.7
1	A	511	GLY	2.6
1	B	228	LYS	2.6
1	A	449	GLY	2.6
1	A	230	ALA	2.6
1	B	140	SER	2.6
1	B	544	LEU	2.6
1	A	520	ASN	2.6
1	B	131	ASP	2.5
1	A	507	LEU	2.5
1	B	60	TRP	2.5
1	B	145	MET	2.5
1	B	260	GLN	2.4
1	C	554	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	133	ALA	2.4
1	A	215	GLN	2.4
1	A	485	LEU	2.4
1	B	128	GLY	2.3
1	B	150	MET	2.3
1	B	557	GLN	2.3
1	B	298	VAL	2.3
1	A	84	PHE	2.3
1	A	510	GLY	2.3
1	B	255	GLY	2.3
1	A	323	VAL	2.3
1	C	58	LEU	2.3
1	B	250	THR	2.3
1	B	146	PHE	2.2
1	A	293	SER	2.2
1	B	303	GLN	2.2
1	A	514	ALA	2.2
1	B	545	SER	2.2
1	B	296	SER	2.2
1	C	229	GLY	2.2
1	A	145	MET	2.2
1	B	136	PHE	2.2
1	A	388	ILE	2.2
1	C	451	GLN	2.1
1	C	509	SER	2.1
1	A	253	SER	2.1
1	C	560	ASN	2.1
1	B	555	GLU	2.1
1	A	297	GLY	2.1
1	A	272	GLU	2.1
1	C	565	ARG	2.1
1	A	62	VAL	2.1
1	A	515	LEU	2.0
1	A	419	THR	2.0
1	A	79	GLY	2.0
1	B	232	GLY	2.0
1	B	268	ALA	2.0
1	A	423	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CHT	C	601	7/7	0.90	0.28	2.99	99,103,112,121	0
3	PGT	A	602	51/51	0.90	0.29	1.92	24,47,72,73	30
2	CL	A	601	1/1	0.93	0.19	0.58	105,105,105,105	0
2	CL	C	602	1/1	0.97	0.11	-1.66	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.