



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 AM UTC

PDB ID : 9G8J / pdb_00009g8j
Title : Structure of K⁺-dependent Na⁺-PPase from *Thermotoga maritima* in complex with zoledronate
Authors : Vidilaseris, K.; Liu, J.; Goldman, A.
Deposited on : 2024-07-23
Resolution : 3.26 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

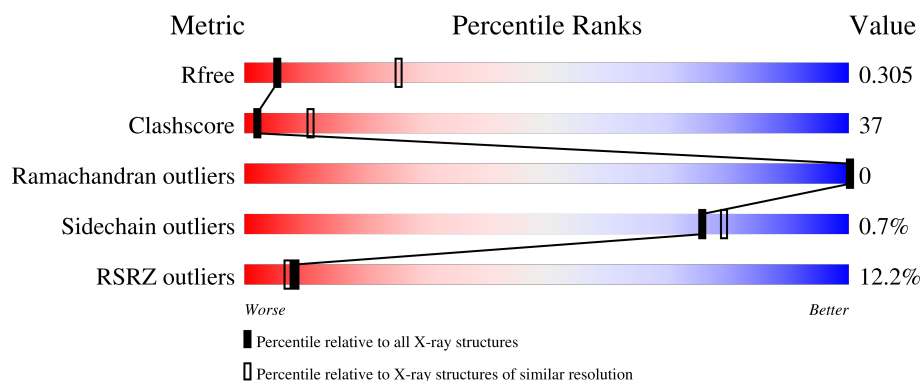
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 $\leq 5\%$. 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	735	12% 47% 51% ..
1	B	735	10% 44% 53% .
1	C	735	13% 50% 47% .
1	D	735	13% 50% 47% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZOL	A	801	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20925 atoms, of which 70 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called K(+)-stimulated pyrophosphate-energized sodium pump.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	0	0
			5238	3430	819	962	27			
1	B	716	Total	C	N	O	S	0	0	0
			5159	3383	804	946	26			
1	C	720	Total	C	N	O	S	0	0	0
			5205	3407	816	955	27			
1	D	716	Total	C	N	O	S	0	0	0
			5128	3359	797	946	26			

There are 48 discrepancies between the modelled and reference sequences:

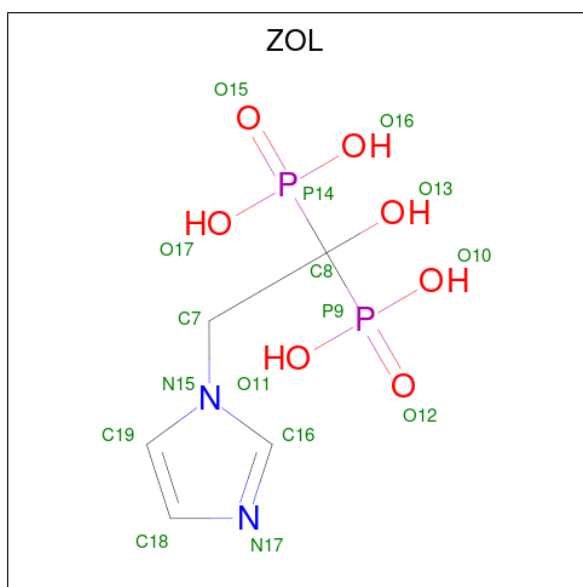
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP Q9S5X0
A	-7	ARG	-	expression tag	UNP Q9S5X0
A	-6	GLY	-	expression tag	UNP Q9S5X0
A	-5	SER	-	expression tag	UNP Q9S5X0
A	-4	HIS	-	expression tag	UNP Q9S5X0
A	-3	HIS	-	expression tag	UNP Q9S5X0
A	-2	HIS	-	expression tag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

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

- Molecule 2 is ZOLEDRONIC ACID (CCD ID: ZOL) (formula: $C_5H_{10}N_2O_7P_2$).

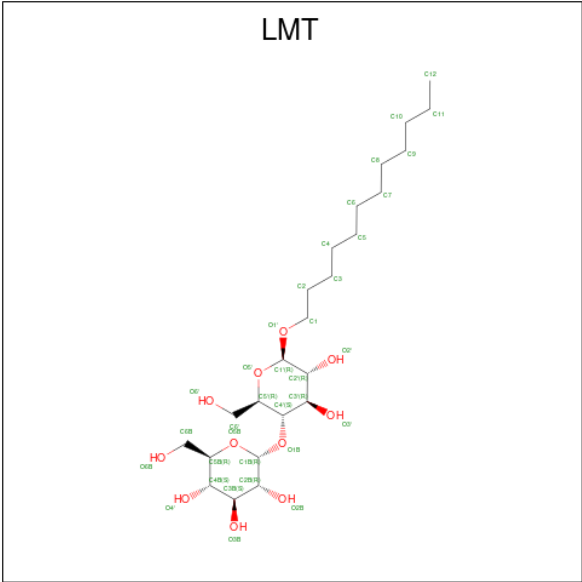


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total 22	C 5	H 6	N 2	O 7	P 2	0	0
2	B	1	Total 22	C 5	H 6	N 2	O 7	P 2	0	0
2	C	1	Total 22	C 5	H 6	N 2	O 7	P 2	0	0
2	D	1	Total 22	C 5	H 6	N 2	O 7	P 2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		
3	B	4	Total	Mg	0	0
			4	4		
3	C	4	Total	Mg	0	0
			4	4		
3	D	4	Total	Mg	0	0
			4	4		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			81	24	46	11		

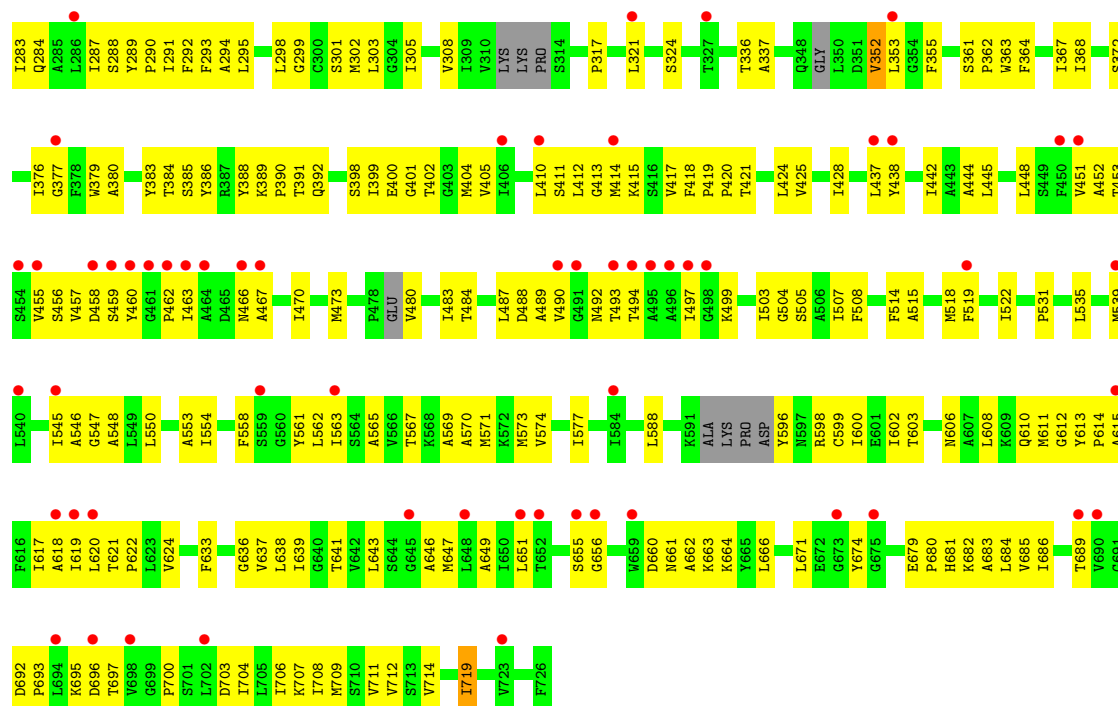
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O	0	0
			2 2		
5	B	8	Total O	0	0
			8 8		

- Chain B: 10% 44% 53%

Sequence logo showing amino acid conservation across 274 positions. The logo is divided into three color-coded regions: red (10% conservation), orange (44% conservation), and yellow (53% conservation). The x-axis represents the position in the chain (1 to 274), and the y-axis represents the amino acid frequency. The logo is composed of many small bars, each representing an amino acid at a specific position. The bars are color-coded by amino acid: A (green), C (blue), D (orange), E (yellow), F (red), G (green), H (blue), I (orange), L (green), M (blue), N (orange), P (yellow), Q (blue), R (red), S (green), T (yellow), V (blue), W (orange), Y (red). The logo shows that the first 10% of the chain (positions 1-27) is highly conserved, with many positions having a single dominant amino acid. The middle 44% (positions 28-121) shows more variability, with many positions having multiple amino acids. The last 53% (positions 122-274) shows the least conservation, with many positions having a single dominant amino acid.

- Chain C:
-
- 13% 50% 47%
- MET ARG GLY SER HIS HIS HIS HIS HIS HIS Y2 F8 L9 I10 P11 L12 V13 A18 V25 VAL R27 K28 P29 R34 I38 Y41 I42 D47 S48 F49 L50 E53 T54 I57 F58 K59 V60 A61 I62 V63 I64 A65 T72 T73 T76 G77 V78 A79



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.19Å 147.36Å 252.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 3.26 48.22 – 3.26	Depositor EDS
% Data completeness (in resolution range)	55.2 (48.22-3.26) 55.4 (48.22-3.26)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.266 , 0.306 0.265 , 0.305	Depositor DCC
R_{free} test set	1673 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	122.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 87.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20925	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, 0.333 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: ZOL, MG, LMT

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	0.38	0/5349	0.58	1/7304 (0.0%)
1	B	0.24	0/5270	0.40	1/7202 (0.0%)
1	C	0.25	0/5313	0.43	1/7251 (0.0%)
1	D	0.25	0/5232	0.42	0/7150
All	All	0.28	0/21164	0.46	3/28907 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	720	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	720	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	720	PHE	CA-CB-CG	5.05	118.85	113.80

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	5238	0	5206	435	0
1	B	5159	0	5110	434	0
1	C	5205	0	5163	358	0
1	D	5128	0	5058	394	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	16	6	6	0	0
2	B	16	6	7	3	0
2	C	16	6	7	0	0
2	D	16	6	7	2	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	D	35	46	46	0	0
5	A	2	0	0	2	0
5	B	8	0	0	6	0
All	All	20855	70	20610	1546	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 37.

All (1546) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:MET:HG2	1:D:128:VAL:HG21	1.27	1.16
1:A:138:LEU:HD13	1:A:295:LEU:HD23	1.29	1.15
1:A:571:MET:HG3	1:B:404:MET:HE2	1.30	1.13
1:B:39:SER:HB2	1:B:103:VAL:HG21	1.31	1.12
1:B:244:LEU:HD23	1:B:455:VAL:HG22	1.31	1.12
1:A:546:ALA:HB1	1:B:425:VAL:HG13	1.30	1.11
1:D:50:LEU:HD21	1:D:92:ILE:HG12	1.23	1.11
1:B:138:LEU:HD13	1:B:295:LEU:HD23	1.24	1.10
1:C:400:GLU:HG3	1:D:571:MET:HG3	1.29	1.10
1:A:39:SER:HB2	1:A:103:VAL:HG11	1.28	1.10
1:C:425:VAL:HG13	1:D:546:ALA:HB1	1.34	1.08
1:D:7:PHE:HB3	1:D:295:LEU:HD13	1.36	1.08
1:C:259:ALA:HA	1:C:262:MET:HE2	1.22	1.07
1:A:503:ILE:HD11	1:A:646:ALA:HA	1.39	1.04
1:C:546:ALA:HB1	1:D:425:VAL:HG13	1.37	1.04
1:C:571:MET:HG3	1:D:404:MET:HE2	1.39	1.03
1:D:201:ALA:HA	1:D:573:MET:HE1	1.41	1.00
1:C:573:MET:HE3	1:C:599:CYS:HB3	1.39	1.00
1:A:240:LEU:HD21	1:A:458:ASP:HB3	1.41	1.00
1:C:530:PRO:HG2	1:C:533:LEU:HD13	1.42	0.99
1:D:220:PRO:HG3	1:D:473:MET:HA	1.45	0.98
1:B:50:LEU:HD21	1:B:92:ILE:HG13	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ILE:HD12	1:A:649:ALA:HB3	1.47	0.96
1:C:377:GLY:HA3	1:C:497:ILE:HG23	1.46	0.96
1:A:581:ALA:HA	1:A:587:LEU:HD11	1.46	0.96
1:C:613:TYR:CE2	1:C:617:ILE:HD11	2.00	0.96
1:B:109:ALA:HB2	1:B:118:ALA:HB2	1.45	0.96
1:A:226:ILE:HG23	1:A:600:ILE:HD11	1.47	0.96
1:D:618:ALA:CB	1:D:708:ILE:HD11	1.95	0.95
1:B:489:ALA:HB2	1:B:664:LYS:HE2	1.48	0.94
1:C:569:ALA:HB2	1:C:606:ASN:HD22	1.32	0.94
1:B:87:SER:HA	1:B:245:LEU:HD23	1.50	0.94
2:B:801:ZOL:O13	5:B:901:HOH:O	1.83	0.94
1:A:507:ILE:HD11	1:A:646:ALA:HB2	1.46	0.93
1:D:50:LEU:HD13	1:D:95:MET:HE2	1.50	0.93
1:A:622:PRO:HG3	1:A:709:MET:HG3	1.50	0.93
1:B:141:LEU:HD21	1:B:252:ILE:HG21	1.50	0.93
1:B:530:PRO:HG2	1:B:533:LEU:HD13	1.49	0.92
1:B:25:VAL:HG11	1:B:124:GLN:HG2	1.52	0.92
1:B:622:PRO:HG3	1:B:709:MET:HG3	1.52	0.91
1:D:184:SER:HA	1:D:246:GLU:HG3	1.50	0.91
1:C:517:TYR:HB2	1:C:714:VAL:HG22	1.49	0.91
1:C:220:PRO:HG3	1:C:473:MET:HA	1.51	0.90
1:D:266:TYR:HD1	1:D:531:PRO:HG2	1.35	0.90
1:B:14:ALA:HB2	1:B:298:LEU:HD21	1.54	0.90
1:B:25:VAL:CG1	1:B:124:GLN:HG2	2.02	0.89
1:D:215:LEU:HD21	1:D:219:ASP:HB3	1.54	0.89
1:C:400:GLU:HG3	1:D:571:MET:CG	2.03	0.88
1:D:444:ALA:HB2	1:D:508:PHE:HB3	1.55	0.88
1:C:522:ILE:HD11	1:C:534:VAL:HG13	1.53	0.88
1:B:103:VAL:HG22	1:B:470:ILE:HD12	1.56	0.88
1:C:191:ARG:HD3	1:C:700:PRO:HB2	1.56	0.88
1:B:94:GLY:HA3	1:B:129:MET:SD	2.14	0.88
1:B:141:LEU:CD2	1:B:252:ILE:HG21	2.04	0.87
1:D:125:GLY:O	1:D:128:VAL:HG22	1.73	0.87
1:A:119:LEU:HD13	1:A:317:PRO:HB3	1.55	0.87
1:D:39:SER:HB2	1:D:103:VAL:HG21	1.56	0.87
1:A:539:MET:HE3	1:B:539:MET:HE3	1.57	0.87
1:B:477:ASP:O	1:B:480:VAL:HG12	1.74	0.86
1:D:185:ILE:CD1	1:D:619:ILE:HD11	2.06	0.86
1:D:191:ARG:HD3	1:D:700:PRO:HB2	1.57	0.86
1:B:244:LEU:HD23	1:B:455:VAL:CG2	2.06	0.85
1:D:573:MET:O	1:D:577:ILE:HG12	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:LEU:HD12	1:D:545:ILE:HD13	1.59	0.84
1:D:215:LEU:HG	1:D:216:PRO:HD2	1.57	0.84
1:B:137:ALA:HB2	1:B:245:LEU:CD1	2.07	0.84
1:C:115:ILE:HG23	1:C:487:LEU:HD11	1.57	0.84
1:C:185:ILE:HD12	1:C:619:ILE:HD11	1.57	0.84
1:D:618:ALA:HB3	1:D:708:ILE:HD11	1.59	0.84
1:B:444:ALA:HB2	1:B:508:PHE:HB3	1.60	0.84
1:A:18:ALA:HB2	1:A:131:LEU:HB2	1.58	0.83
1:B:321:LEU:HD13	1:B:457:VAL:HG13	1.59	0.83
1:A:223:PRO:HG2	1:A:577:ILE:HD12	1.60	0.83
1:A:39:SER:HB2	1:A:103:VAL:CG1	2.08	0.83
1:C:539:MET:HG2	1:D:639:ILE:HD13	1.59	0.83
1:C:225:THR:HB	1:C:473:MET:HE1	1.61	0.83
1:C:540:LEU:HD21	1:D:518:MET:HG3	1.59	0.83
1:D:618:ALA:HB1	1:D:708:ILE:HD11	1.61	0.83
1:C:569:ALA:HB2	1:C:606:ASN:ND2	1.94	0.82
1:A:573:MET:HE2	1:A:603:THR:HG23	1.62	0.82
1:D:43:ARG:HG3	1:D:99:THR:HB	1.62	0.82
1:D:163:ASN:OD1	1:D:167:ILE:HB	1.79	0.82
1:A:233:ASN:O	1:A:237:VAL:HB	1.79	0.82
1:A:446:GLY:HA2	1:A:449:SER:OG	1.79	0.82
1:B:519:PHE:HE1	1:B:535:LEU:HD21	1.45	0.82
1:B:184:SER:HA	1:B:246:GLU:HG3	1.62	0.81
1:B:663:LYS:HA	1:B:684:LEU:HD23	1.60	0.81
1:B:112:THR:HG23	1:B:114:LYS:H	1.44	0.81
1:D:223:PRO:HG2	1:D:577:ILE:HD12	1.61	0.81
1:A:647:MET:HE1	1:B:553:ALA:HA	1.60	0.81
1:A:661:ASN:ND2	5:A:901:HOH:O	2.13	0.81
1:C:84:ALA:HB1	1:C:186:ILE:HD12	1.63	0.81
1:D:685:VAL:O	1:D:689:THR:HG23	1.81	0.81
1:B:129:MET:HE3	1:B:241:GLY:HA3	1.60	0.81
1:A:270:ILE:HD12	1:A:275:VAL:HG21	1.62	0.81
1:B:221:ARG:HD3	1:B:590:GLY:HA2	1.63	0.81
1:B:308:VAL:HG21	1:B:324:SER:HB2	1.63	0.81
1:A:120:LYS:O	1:A:124:GLN:HG2	1.81	0.80
1:A:639:ILE:HD13	1:B:539:MET:HG2	1.62	0.80
1:A:184:SER:HA	1:A:246:GLU:HG3	1.62	0.80
1:A:194:GLY:HA3	1:A:235:GLY:HA2	1.63	0.80
1:B:647:MET:HE2	1:B:647:MET:HA	1.63	0.80
1:D:437:LEU:HD13	1:D:515:ALA:HB2	1.64	0.80
1:B:65:ALA:CB	1:B:81:LEU:HD21	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:HD13	1:B:708:ILE:HD11	1.63	0.80
1:D:414:MET:HG2	1:D:651:LEU:HD11	1.64	0.79
1:C:414:MET:HG2	1:C:651:LEU:HD11	1.64	0.79
2:B:801:ZOL:O11	5:B:902:HOH:O	2.01	0.79
1:C:84:ALA:HB1	1:C:186:ILE:CD1	2.13	0.79
1:D:176:VAL:HB	1:D:253:VAL:HG13	1.63	0.79
1:A:223:PRO:HG2	1:A:577:ILE:CD1	2.12	0.79
1:D:174:MET:HE2	1:D:174:MET:HA	1.65	0.79
1:B:115:ILE:HG12	1:B:483:ILE:HG23	1.65	0.78
1:A:138:LEU:HD12	1:A:298:LEU:HD13	1.64	0.78
1:C:258:LEU:O	1:C:262:MET:HG3	1.84	0.78
1:C:639:ILE:HD13	1:D:539:MET:SD	2.24	0.78
1:B:39:SER:CB	1:B:103:VAL:HG21	2.12	0.78
1:D:421:THR:HG22	1:D:647:MET:HE1	1.66	0.77
1:B:635:GLY:O	1:B:639:ILE:HD12	1.84	0.77
1:D:385:SER:HA	1:D:661:ASN:ND2	2.00	0.77
1:D:256:ILE:HG23	1:D:287:ILE:HG23	1.65	0.77
1:B:53:GLU:O	1:B:57:ILE:HG23	1.83	0.77
1:B:163:ASN:OD1	1:B:167:ILE:HB	1.83	0.77
1:C:685:VAL:O	1:C:689:THR:HG23	1.85	0.77
1:D:656:GLY:HA3	1:D:695:LYS:HG3	1.67	0.77
1:B:181:LEU:O	1:B:185:ILE:HG12	1.85	0.77
1:B:376:ILE:HD11	1:B:424:LEU:HD21	1.67	0.77
1:C:337:ALA:HB2	1:C:363:TRP:CZ2	2.20	0.76
1:D:385:SER:HA	1:D:661:ASN:HD22	1.49	0.76
1:B:129:MET:CE	1:B:241:GLY:HA3	2.14	0.76
1:C:105:VAL:HG23	1:C:467:ALA:HB2	1.67	0.76
1:C:666:LEU:HD22	1:C:681:HIS:HD2	1.49	0.76
1:B:53:GLU:OE2	1:B:190:ASP:HA	1.85	0.76
1:B:695:LYS:NZ	5:B:902:HOH:O	2.17	0.76
1:C:199:LYS:HE3	1:C:696:ASP:HB2	1.67	0.76
1:D:266:TYR:CD1	1:D:531:PRO:HG2	2.21	0.76
1:C:598:ARG:O	1:C:602:ILE:HG12	1.85	0.75
1:D:261:TYR:O	1:D:265:ILE:HG12	1.86	0.75
1:A:65:ALA:CB	1:A:81:LEU:HD21	2.16	0.75
1:B:414:MET:HG2	1:B:651:LEU:HD11	1.66	0.75
1:C:363:TRP:CZ2	1:C:367:ILE:HD11	2.22	0.75
1:D:308:VAL:HG21	1:D:324:SER:HB2	1.67	0.75
1:B:23:ALA:O	1:B:26:VAL:HG12	1.87	0.75
1:D:185:ILE:HD13	1:D:619:ILE:HD11	1.69	0.75
1:A:149:GLY:HA3	1:A:155:VAL:HG13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ASN:OD1	1:C:158:LEU:N	2.20	0.74
1:D:31:GLY:H	1:D:107:GLU:HB2	1.52	0.74
1:D:240:LEU:HD21	1:D:458:ASP:HB3	1.70	0.74
1:A:82:LEU:O	1:A:86:MET:HG2	1.87	0.74
1:B:596:TYR:O	1:B:600:ILE:HG12	1.87	0.74
1:B:21:ASN:O	1:B:25:VAL:HG22	1.87	0.74
1:A:425:VAL:HG13	1:B:546:ALA:HB1	1.69	0.74
1:B:336:THR:HG22	1:B:363:TRP:HD1	1.51	0.74
1:D:157:ASN:OD1	1:D:158:LEU:N	2.20	0.74
1:B:671:LEU:HD22	1:B:674:TYR:HB2	1.67	0.74
1:A:129:MET:HE1	1:A:237:VAL:O	1.87	0.74
1:B:444:ALA:HB2	1:B:508:PHE:CB	2.18	0.74
1:B:299:GLY:HA2	1:B:302:MET:HE2	1.69	0.74
1:B:503:ILE:HD13	1:B:703:ASP:HB3	1.69	0.74
1:C:666:LEU:HD22	1:C:681:HIS:CD2	2.23	0.73
1:D:215:LEU:HD23	1:D:216:PRO:O	1.86	0.73
1:D:363:TRP:CZ2	1:D:367:ILE:HD11	2.22	0.73
1:D:226:ILE:HG21	1:D:596:TYR:HB3	1.70	0.73
1:A:21:ASN:HB3	1:A:128:VAL:CG2	2.18	0.73
1:A:573:MET:HE1	1:A:599:CYS:HB3	1.69	0.73
1:C:622:PRO:HG3	1:C:709:MET:HG3	1.70	0.73
1:C:425:VAL:HG21	1:D:550:LEU:CD2	2.18	0.73
1:A:265:ILE:HD11	1:A:522:ILE:HD13	1.71	0.73
1:C:380:ALA:O	1:C:384:THR:HG22	1.89	0.73
1:D:143:LEU:O	1:D:147:ILE:HG12	1.89	0.73
1:B:21:ASN:HB3	1:B:124:GLN:CD	2.14	0.73
1:B:207:LEU:HD12	1:B:689:THR:HG21	1.71	0.72
1:A:157:ASN:OD1	1:A:158:LEU:N	2.20	0.72
1:C:72:THR:HB	1:C:174:MET:HE2	1.71	0.72
1:C:8:PHE:HE2	1:C:146:LEU:HD21	1.54	0.72
1:B:233:ASN:O	1:B:237:VAL:HB	1.90	0.72
1:D:201:ALA:HA	1:D:573:MET:CE	2.17	0.72
1:D:444:ALA:HB2	1:D:508:PHE:CB	2.19	0.72
1:C:184:SER:HA	1:C:246:GLU:HG3	1.71	0.72
1:A:176:VAL:HG22	1:A:253:VAL:HG13	1.71	0.72
1:B:27:ARG:HG3	1:B:29:PRO:HD3	1.72	0.72
1:A:299:GLY:HA2	1:A:302:MET:CE	2.20	0.72
1:A:538:ASN:HB2	1:B:536:LEU:HD13	1.71	0.72
1:A:573:MET:O	1:A:577:ILE:HG12	1.90	0.72
1:A:208:VAL:HG21	1:A:577:ILE:HG21	1.71	0.72
1:A:448:LEU:HD23	1:A:448:LEU:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:MET:SD	1:A:599:CYS:HB3	2.30	0.72
1:C:256:ILE:HG23	1:C:287:ILE:HG23	1.71	0.72
1:C:400:GLU:CG	1:D:571:MET:HG3	2.13	0.72
1:D:90:ALA:HB2	1:D:136:PHE:HD2	1.55	0.72
1:D:106:ALA:HB2	1:D:467:ALA:HB1	1.69	0.72
1:D:499:LYS:O	1:D:503:ILE:HD12	1.89	0.72
1:A:116:GLY:O	1:A:120:LYS:HG2	1.90	0.71
1:A:199:LYS:HE3	1:A:696:ASP:HB2	1.71	0.71
1:C:262:MET:SD	1:C:353:LEU:HD22	2.30	0.71
1:A:105:VAL:HA	1:A:121:VAL:HG11	1.71	0.71
1:C:533:LEU:O	1:C:536:LEU:HD22	1.91	0.71
1:D:380:ALA:O	1:D:384:THR:HG22	1.90	0.71
1:C:425:VAL:CG1	1:D:546:ALA:HB1	2.16	0.71
1:D:514:PHE:CE1	1:D:638:LEU:HB3	2.24	0.71
1:C:444:ALA:HB2	1:C:508:PHE:HB3	1.72	0.71
1:D:194:GLY:HA2	1:D:234:VAL:HG12	1.71	0.71
1:A:227:ALA:HB2	1:A:600:ILE:HD13	1.72	0.71
1:B:82:LEU:O	1:B:86:MET:HG2	1.90	0.71
1:B:107:GLU:OE2	1:B:110:ARG:NH2	2.23	0.71
1:C:8:PHE:CE2	1:C:146:LEU:HD21	2.25	0.71
1:A:30:GLU:OE1	1:A:36:LYS:HG2	1.90	0.71
1:A:300:CYS:SG	1:A:331:LEU:HB2	2.31	0.71
1:A:448:LEU:CD2	1:A:451:VAL:HB	2.21	0.71
1:A:553:ALA:HB2	1:B:421:THR:HG21	1.72	0.71
1:B:21:ASN:HB3	1:B:124:GLN:OE1	1.91	0.71
1:A:199:LYS:HG3	1:A:693:PRO:HA	1.72	0.71
1:C:120:LYS:HD2	1:C:313:PRO:HD3	1.71	0.71
1:B:363:TRP:CZ2	1:B:367:ILE:HD11	2.25	0.71
1:C:42:ILE:HG23	1:C:230:VAL:HG12	1.72	0.71
1:C:573:MET:CE	1:C:599:CYS:HB3	2.20	0.71
1:A:571:MET:HE3	1:B:400:GLU:HG3	1.73	0.71
1:B:550:LEU:HD13	1:B:633:PHE:HZ	1.55	0.71
1:C:402:THR:HA	1:C:683:ALA:HB1	1.73	0.71
1:A:210:LYS:CE	1:A:217:GLU:HB2	2.21	0.70
1:A:176:VAL:HG13	1:A:257:ILE:HD11	1.71	0.70
1:B:49:PHE:CD2	1:B:234:VAL:HG11	2.26	0.70
1:C:639:ILE:HG21	1:D:539:MET:SD	2.32	0.70
1:B:451:VAL:O	1:B:455:VAL:HG23	1.90	0.70
1:B:494:THR:O	1:B:497:ILE:HG12	1.91	0.70
1:B:87:SER:HA	1:B:245:LEU:CD2	2.21	0.70
1:B:489:ALA:HB2	1:B:664:LYS:CE	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PHE:HB2	1:A:283:ILE:HG13	1.74	0.70
1:A:191:ARG:HD3	1:A:700:PRO:HB2	1.72	0.70
1:B:226:ILE:O	1:B:230:VAL:HG12	1.92	0.70
1:C:425:VAL:HG13	1:D:546:ALA:CB	2.18	0.70
1:C:191:ARG:HH21	1:C:240:LEU:HA	1.57	0.70
1:A:82:LEU:HD23	1:A:144:VAL:HG23	1.73	0.70
1:A:321:LEU:HD22	1:A:457:VAL:HG22	1.74	0.70
1:A:598:ARG:O	1:A:602:ILE:HG12	1.91	0.70
1:A:207:LEU:O	1:A:211:THR:HG22	1.92	0.69
1:A:563:ILE:HG22	1:B:411:SER:HB2	1.74	0.69
1:D:615:ALA:O	1:D:619:ILE:HG13	1.92	0.69
1:B:492:ASN:HB2	5:B:908:HOH:O	1.92	0.69
1:C:304:GLY:O	1:C:308:VAL:HG23	1.91	0.69
1:D:308:VAL:CG2	1:D:324:SER:HB2	2.22	0.69
1:D:184:SER:CA	1:D:246:GLU:HG3	2.20	0.69
1:B:386:TYR:HA	1:B:391:THR:HB	1.74	0.69
1:B:337:ALA:HB2	1:B:363:TRP:CZ2	2.26	0.69
1:B:75:GLN:HA	1:B:78:VAL:HG12	1.73	0.69
1:B:109:ALA:HB2	1:B:118:ALA:CB	2.23	0.69
1:C:81:LEU:O	1:C:85:VAL:HG23	1.92	0.69
1:C:444:ALA:HB2	1:C:508:PHE:CB	2.22	0.69
1:A:199:LYS:CE	1:A:696:ASP:HB2	2.23	0.69
1:A:226:ILE:CG2	1:A:596:TYR:HB3	2.23	0.69
1:C:318:GLN:HB3	1:C:490:VAL:HG11	1.75	0.69
1:C:377:GLY:CA	1:C:497:ILE:HG23	2.23	0.69
1:D:608:LEU:HA	1:D:611:MET:HE3	1.74	0.69
1:A:149:GLY:O	1:A:155:VAL:HG22	1.93	0.69
1:C:49:PHE:CD2	1:C:234:VAL:HG21	2.28	0.69
1:C:547:GLY:O	1:C:637:VAL:HA	1.93	0.69
1:A:511:LEU:HD12	1:B:545:ILE:HD13	1.74	0.68
1:C:181:LEU:O	1:C:185:ILE:HG12	1.92	0.68
1:C:597:ASN:HA	1:C:600:ILE:HG12	1.75	0.68
1:B:217:GLU:O	1:B:472:GLU:HG2	1.94	0.68
1:C:411:SER:HB2	1:D:563:ILE:HG22	1.75	0.68
1:C:563:ILE:O	1:C:567:THR:HG23	1.94	0.68
1:D:247:SER:HA	1:D:707:LYS:HE3	1.74	0.68
1:B:213:LEU:CB	1:B:215:LEU:HD13	2.24	0.68
1:C:543:ARG:NH1	1:C:629:LEU:O	2.26	0.68
1:D:7:PHE:HB3	1:D:295:LEU:CD1	2.18	0.68
1:A:622:PRO:CG	1:A:709:MET:HG3	2.23	0.68
1:C:263:PHE:HB2	1:C:283:ILE:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HG2	1:A:312:LYS:H	1.59	0.68
1:A:444:ALA:HB2	1:A:508:PHE:HB3	1.76	0.68
1:B:75:GLN:O	1:B:78:VAL:HG12	1.94	0.68
1:A:573:MET:CE	1:A:599:CYS:HB3	2.23	0.68
1:C:393:PHE:CZ	1:D:571:MET:HE1	2.28	0.68
1:A:299:GLY:HA2	1:A:302:MET:HE2	1.76	0.68
1:C:521:GLN:HG2	1:C:717:VAL:HG21	1.77	0.67
1:D:420:PRO:O	1:D:424:LEU:HD23	1.94	0.67
1:A:188:MET:HE2	1:A:704:ILE:HG22	1.74	0.67
1:D:82:LEU:O	1:D:86:MET:HG2	1.94	0.67
1:A:154:GLN:OE1	1:A:171:PRO:HB3	1.94	0.67
1:C:185:ILE:HD13	1:C:708:ILE:HD11	1.74	0.67
1:D:148:PHE:O	1:D:152:MET:HB2	1.94	0.67
1:D:608:LEU:HD23	1:D:611:MET:HE3	1.76	0.67
1:A:97:MET:HE3	1:A:128:VAL:HG21	1.77	0.67
1:D:97:MET:HG2	1:D:128:VAL:CG2	2.17	0.67
1:B:398:SER:HA	1:B:405:VAL:CG2	2.25	0.67
1:A:199:LYS:HD2	1:A:692:ASP:HB3	1.75	0.67
1:D:337:ALA:HB2	1:D:363:TRP:CZ2	2.30	0.67
1:B:667:GLU:OE1	5:B:903:HOH:O	2.12	0.66
1:D:547:GLY:O	1:D:637:VAL:HA	1.94	0.66
1:B:446:GLY:HA2	1:B:449:SER:OG	1.95	0.66
1:B:613:TYR:CE2	1:B:617:ILE:HD11	2.30	0.66
1:D:565:ALA:HB2	1:D:610:GLN:OE1	1.95	0.66
1:A:522:ILE:HD11	1:A:534:VAL:CG2	2.24	0.66
1:C:129:MET:HE3	1:C:133:VAL:HG23	1.78	0.66
1:C:621:THR:HB	1:C:622:PRO:HD3	1.77	0.66
1:A:451:VAL:O	1:A:455:VAL:HG22	1.94	0.66
1:D:421:THR:CG2	1:D:647:MET:HE1	2.24	0.66
1:D:437:LEU:HD13	1:D:515:ALA:CB	2.25	0.66
1:A:14:ALA:HB2	1:A:298:LEU:HD21	1.78	0.66
1:B:25:VAL:HG11	1:B:124:GLN:CG	2.26	0.66
1:C:411:SER:HB2	1:D:563:ILE:CG2	2.24	0.66
1:A:471:SER:HA	1:A:476:LEU:HD12	1.78	0.66
1:D:317:PRO:O	1:D:321:LEU:HG	1.96	0.66
1:C:127:SER:HB2	1:C:305:ILE:HG21	1.76	0.66
1:C:129:MET:CE	1:C:241:GLY:HA3	2.25	0.66
1:D:21:ASN:HB2	1:D:128:VAL:HG12	1.78	0.65
1:C:308:VAL:HG22	1:C:324:SER:OG	1.96	0.65
1:C:530:PRO:CG	1:C:533:LEU:HD13	2.22	0.65
1:A:521:GLN:HG2	1:A:717:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ALA:O	1:B:384:THR:HG22	1.95	0.65
1:A:503:ILE:HD11	1:A:646:ALA:CA	2.24	0.65
1:B:84:ALA:HB1	1:B:186:ILE:HG13	1.77	0.65
1:D:115:ILE:HG13	1:D:483:ILE:HG23	1.79	0.65
1:A:185:ILE:HD12	1:A:619:ILE:HD11	1.78	0.65
1:D:226:ILE:CG2	1:D:596:TYR:HB3	2.25	0.65
1:A:18:ALA:HB2	1:A:131:LEU:CB	2.26	0.65
1:A:263:PHE:HB2	1:A:283:ILE:HG21	1.78	0.65
1:A:265:ILE:HD11	1:A:522:ILE:CD1	2.26	0.65
1:C:692:ASP:HA	1:C:695:LYS:HE3	1.78	0.65
1:B:65:ALA:HB2	1:B:81:LEU:HD21	1.78	0.65
1:C:553:ALA:HB2	1:D:421:THR:HG21	1.79	0.65
1:D:97:MET:HE2	1:D:128:VAL:HG11	1.79	0.65
1:D:194:GLY:O	1:D:198:THR:HG22	1.97	0.65
1:A:244:LEU:CD2	1:A:455:VAL:HG12	2.27	0.65
1:A:584:ILE:O	1:A:587:LEU:HD22	1.97	0.65
1:B:185:ILE:HD13	1:B:708:ILE:CD1	2.26	0.65
1:C:138:LEU:HD13	1:C:295:LEU:HD23	1.79	0.65
1:D:622:PRO:HG3	1:D:709:MET:HG3	1.77	0.65
1:B:291:ILE:O	1:B:295:LEU:HG	1.97	0.64
1:C:199:LYS:HD2	1:C:692:ASP:HB3	1.78	0.64
1:B:548:ALA:HA	1:B:636:GLY:O	1.97	0.64
1:B:613:TYR:CD2	1:B:617:ILE:HD11	2.33	0.64
1:D:204:ALA:O	1:D:208:VAL:HG12	1.97	0.64
1:A:459:SER:O	1:A:462:PRO:HD2	1.97	0.64
1:C:137:ALA:HB2	1:C:245:LEU:HG	1.78	0.64
1:A:304:GLY:O	1:A:308:VAL:HG23	1.96	0.64
1:B:157:ASN:HB3	1:B:161:TYR:OH	1.97	0.64
1:C:410:LEU:O	1:C:414:MET:HG3	1.97	0.64
1:A:81:LEU:O	1:A:85:VAL:HG23	1.97	0.64
1:A:296:VAL:HG21	1:A:339:LEU:HD22	1.80	0.64
1:B:246:GLU:OE2	1:B:707:LYS:HE2	1.97	0.64
1:B:514:PHE:CE2	1:B:639:ILE:HG13	2.32	0.64
1:B:685:VAL:O	1:B:689:THR:HG23	1.98	0.64
1:C:376:ILE:HD11	1:C:424:LEU:HG	1.79	0.64
1:D:185:ILE:HD11	1:D:619:ILE:HD11	1.80	0.64
1:D:246:GLU:OE1	1:D:707:LYS:HE2	1.98	0.64
1:A:308:VAL:HG21	1:A:324:SER:HB2	1.80	0.64
1:B:126:GLY:O	1:B:456:SER:HA	1.98	0.64
1:C:323:ILE:O	1:C:327:THR:HG23	1.97	0.64
1:D:222:ASN:HB3	1:D:225:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:CZ	1:A:294:ALA:HB1	2.33	0.64
1:A:587:LEU:HD23	1:A:588:LEU:HD12	1.78	0.64
1:D:280:LYS:O	1:D:284:GLN:HG3	1.98	0.64
1:B:82:LEU:HD23	1:B:144:VAL:HG23	1.80	0.63
1:B:137:ALA:HB2	1:B:245:LEU:HD12	1.81	0.63
1:D:54:THR:HA	1:D:57:ILE:HG12	1.80	0.63
1:A:291:ILE:O	1:A:295:LEU:HG	1.98	0.63
1:D:291:ILE:O	1:D:295:LEU:HG	1.98	0.63
1:A:220:PRO:HD3	1:A:473:MET:HA	1.81	0.63
1:A:204:ALA:O	1:A:208:VAL:HG22	1.98	0.63
1:B:420:PRO:O	1:B:424:LEU:HD23	1.98	0.63
1:B:598:ARG:O	1:B:602:ILE:HG12	1.98	0.63
1:D:122:ALA:HB1	1:D:460:TYR:HD1	1.64	0.63
1:B:108:ALA:O	1:B:112:THR:HG22	1.99	0.63
1:B:365:SER:HB3	1:B:442:ILE:CG2	2.28	0.63
1:D:321:LEU:HD22	1:D:457:VAL:HG22	1.81	0.63
1:D:666:LEU:HD22	1:D:681:HIS:HD2	1.64	0.63
1:D:460:TYR:OH	1:D:487:LEU:HD22	1.98	0.63
1:B:159:ASN:HB2	1:B:161:TYR:HE1	1.62	0.63
1:B:467:ALA:O	1:B:470:ILE:HG22	1.98	0.63
1:C:18:ALA:HB2	1:C:131:LEU:HB2	1.80	0.63
1:A:270:ILE:HD12	1:A:275:VAL:CG2	2.27	0.62
1:A:550:LEU:O	1:A:554:ILE:HG13	1.98	0.62
1:C:57:ILE:CG2	1:C:186:ILE:HG12	2.28	0.62
1:A:248:PHE:HZ	1:A:294:ALA:HB1	1.65	0.62
1:A:251:ALA:HB1	1:A:445:LEU:HA	1.80	0.62
1:A:329:ALA:O	1:A:333:VAL:HG23	1.99	0.62
1:A:418:PHE:HA	1:B:553:ALA:HB1	1.80	0.62
1:C:336:THR:HG22	1:C:363:TRP:HD1	1.64	0.62
1:C:425:VAL:HG21	1:D:550:LEU:HD22	1.81	0.62
1:D:663:LYS:HA	1:D:684:LEU:HD21	1.80	0.62
1:B:615:ALA:O	1:B:619:ILE:HG13	2.00	0.62
1:C:222:ASN:HB3	1:C:225:THR:HG23	1.79	0.62
1:D:244:LEU:CD2	1:D:455:VAL:HG22	2.28	0.62
1:D:613:TYR:O	1:D:617:ILE:HG13	1.99	0.62
1:A:8:PHE:CE2	1:A:146:LEU:HD21	2.34	0.62
1:A:674:TYR:CD2	1:A:680:PRO:HG2	2.34	0.62
1:C:424:LEU:HD13	1:C:507:ILE:HD12	1.81	0.62
1:C:84:ALA:CB	1:C:186:ILE:HD12	2.28	0.62
1:C:301:SER:OG	1:C:452:ALA:HB3	2.00	0.62
1:A:205:ALA:HB2	1:A:224:ALA:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASP:OD1	1:B:220:PRO:HD2	2.00	0.62
1:A:74:TRP:O	1:A:78:VAL:HG23	2.00	0.62
1:A:130:GLY:HA2	1:A:455:VAL:CG2	2.30	0.62
1:B:77:GLY:O	1:B:81:LEU:HD23	2.00	0.62
1:C:197:TYR:CE2	1:C:603:THR:HG23	2.34	0.62
1:D:337:ALA:HB2	1:D:363:TRP:CE2	2.35	0.62
1:A:414:MET:HG2	1:A:651:LEU:HD11	1.81	0.62
1:A:563:ILE:O	1:A:567:THR:HG23	1.99	0.62
1:B:248:PHE:HA	1:B:448:LEU:HD23	1.82	0.62
1:B:203:MET:SD	1:B:693:PRO:HD3	2.40	0.61
1:C:330:LEU:HD12	1:C:331:LEU:N	2.15	0.61
1:D:13:VAL:HG12	1:D:302:MET:HE1	1.81	0.61
1:A:503:ILE:CD1	1:A:649:ALA:HB3	2.28	0.61
1:B:376:ILE:HD11	1:B:424:LEU:CD2	2.30	0.61
1:C:622:PRO:CG	1:C:709:MET:HG3	2.30	0.61
1:A:97:MET:HE3	1:A:128:VAL:CB	2.30	0.61
1:A:458:ASP:O	1:A:462:PRO:HD3	2.00	0.61
1:A:226:ILE:O	1:A:230:VAL:HG22	2.00	0.61
1:A:663:LYS:CA	1:A:684:LEU:HD12	2.31	0.61
1:C:82:LEU:O	1:C:86:MET:HG2	2.01	0.61
1:C:252:ILE:O	1:C:256:ILE:HG13	2.00	0.61
1:C:425:VAL:HG11	1:D:550:LEU:HD23	1.82	0.61
1:A:53:GLU:O	1:A:57:ILE:HG13	2.01	0.61
1:B:459:SER:O	1:B:462:PRO:HD2	2.00	0.61
1:D:10:ILE:HG22	1:D:298:LEU:HD22	1.82	0.61
1:D:86:MET:HE1	1:D:139:LEU:HD23	1.82	0.61
1:D:215:LEU:HD21	1:D:219:ASP:CB	2.28	0.61
1:D:244:LEU:HD23	1:D:455:VAL:HG22	1.83	0.61
1:A:226:ILE:HG21	1:A:596:TYR:HB3	1.81	0.61
1:A:280:LYS:O	1:A:284:GLN:HG3	2.00	0.61
1:B:110:ARG:HG3	1:B:476:LEU:HD21	1.83	0.61
1:B:530:PRO:CG	1:B:533:LEU:HD13	2.27	0.61
1:C:84:ALA:C	1:C:186:ILE:HD12	2.26	0.61
1:D:448:LEU:HD13	1:D:505:SER:HB2	1.83	0.61
1:C:84:ALA:CA	1:C:186:ILE:HD12	2.31	0.61
1:C:459:SER:O	1:C:462:PRO:HD2	2.01	0.61
1:A:298:LEU:HD23	1:A:302:MET:HE2	1.82	0.61
1:C:390:PRO:HB2	1:C:412:LEU:HD11	1.81	0.61
1:D:184:SER:HB3	1:D:708:ILE:HG22	1.82	0.61
1:D:596:TYR:O	1:D:600:ILE:HG12	2.01	0.61
1:A:503:ILE:HD13	1:A:650:ILE:HG13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LYS:N	1:A:684:LEU:HD12	2.16	0.60
1:C:588:LEU:HD12	1:C:588:LEU:H	1.65	0.60
1:D:246:GLU:OE1	1:D:704:ILE:HD13	2.01	0.60
1:A:621:THR:HB	1:A:622:PRO:HD3	1.83	0.60
1:B:480:VAL:HG13	1:B:481:ARG:N	2.16	0.60
1:C:94:GLY:HA3	1:C:129:MET:SD	2.40	0.60
1:D:410:LEU:O	1:D:414:MET:HG3	2.01	0.60
1:D:662:ALA:O	1:D:684:LEU:HD21	2.01	0.60
1:D:663:LYS:HA	1:D:684:LEU:CD2	2.30	0.60
1:A:308:VAL:HG21	1:A:324:SER:CB	2.30	0.60
1:A:444:ALA:HB2	1:A:508:PHE:CB	2.30	0.60
1:B:336:THR:HG22	1:B:363:TRP:CD1	2.36	0.60
1:D:336:THR:HG22	1:D:363:TRP:HD1	1.65	0.60
1:A:693:PRO:O	1:A:697:THR:HB	2.02	0.60
1:B:252:ILE:HD13	1:B:445:LEU:HD22	1.83	0.60
1:B:321:LEU:HD13	1:B:457:VAL:CG1	2.31	0.60
1:C:119:LEU:CD2	1:C:317:PRO:HB2	2.31	0.60
1:B:102:ASN:OD1	1:B:103:VAL:N	2.33	0.60
1:C:663:LYS:HB2	1:C:684:LEU:HD22	1.84	0.60
1:D:647:MET:HA	1:D:647:MET:HE2	1.82	0.60
1:B:489:ALA:CB	1:B:664:LYS:HE2	2.27	0.60
1:C:344:LEU:HB2	1:C:359:ALA:HB1	1.83	0.60
1:D:483:ILE:O	1:D:487:LEU:HG	2.02	0.60
1:A:548:ALA:HA	1:A:636:GLY:O	2.01	0.60
1:C:141:LEU:HD21	1:C:252:ILE:HG21	1.82	0.60
1:A:5:ALA:O	1:A:9:LEU:HD23	2.01	0.60
1:A:112:THR:HG21	1:A:117:PRO:HG2	1.83	0.60
1:A:573:MET:CE	1:A:603:THR:HG23	2.31	0.60
1:B:81:LEU:O	1:B:85:VAL:HG23	2.02	0.60
1:B:663:LYS:HD2	1:B:685:VAL:HG22	1.83	0.60
1:D:102:ASN:OD1	1:D:103:VAL:N	2.34	0.60
1:D:421:THR:O	1:D:425:VAL:HG23	2.01	0.60
1:B:421:THR:CG2	1:B:647:MET:HE1	2.31	0.60
1:B:561:TYR:CE2	1:B:614:PRO:HD3	2.35	0.60
1:C:336:THR:HG22	1:C:363:TRP:CD1	2.37	0.60
1:C:421:THR:HG21	1:D:553:ALA:HB2	1.83	0.60
1:C:571:MET:HG3	1:D:404:MET:CE	2.24	0.60
1:A:21:ASN:HB3	1:A:128:VAL:HG23	1.84	0.59
1:A:301:SER:O	1:A:305:ILE:HG23	2.02	0.59
1:B:621:THR:HB	1:B:622:PRO:HD3	1.84	0.59
1:D:138:LEU:HD12	1:D:295:LEU:CD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD23	1:A:144:VAL:CG2	2.32	0.59
1:A:438:TYR:O	1:A:442:ILE:HG12	2.02	0.59
1:A:587:LEU:CD2	1:A:588:LEU:HD12	2.31	0.59
1:B:561:TYR:HE2	1:B:614:PRO:HD3	1.65	0.59
1:D:30:GLU:HA	1:D:107:GLU:OE1	2.02	0.59
1:D:417:VAL:O	1:D:421:THR:HG23	2.02	0.59
1:D:570:ALA:O	1:D:574:VAL:HG23	2.02	0.59
1:A:615:ALA:O	1:A:619:ILE:HG13	2.02	0.59
1:C:247:SER:HA	1:C:707:LYS:HE3	1.84	0.59
1:C:571:MET:CG	1:D:404:MET:HE2	2.25	0.59
1:D:372:SER:O	1:D:376:ILE:HG13	2.01	0.59
1:A:398:SER:HB3	1:A:684:LEU:HD21	1.84	0.59
1:B:329:ALA:O	1:B:333:VAL:HG23	2.03	0.59
1:B:622:PRO:HB3	1:B:713:SER:OG	2.01	0.59
1:C:386:TYR:HA	1:C:391:THR:HB	1.84	0.59
1:D:674:TYR:CD2	1:D:680:PRO:HG2	2.37	0.59
1:D:438:TYR:O	1:D:442:ILE:HG12	2.02	0.59
1:A:252:ILE:O	1:A:256:ILE:HG12	2.02	0.59
1:B:161:TYR:O	1:B:168:ASN:HA	2.02	0.59
1:B:419:PRO:HB2	1:B:420:PRO:HD3	1.82	0.59
1:C:327:THR:HA	1:C:330:LEU:CD2	2.33	0.59
1:A:547:GLY:O	1:A:637:VAL:HA	2.02	0.59
1:B:337:ALA:HB2	1:B:363:TRP:CE2	2.38	0.59
1:A:511:LEU:HD11	1:B:545:ILE:HG21	1.84	0.59
1:B:25:VAL:CG2	1:B:97:MET:HE1	2.32	0.59
1:B:137:ALA:HB2	1:B:245:LEU:HD11	1.84	0.59
1:C:419:PRO:HB2	1:C:420:PRO:HD3	1.84	0.59
1:D:131:LEU:CD2	1:D:302:MET:HG2	2.32	0.59
1:B:46:ALA:HB2	1:B:230:VAL:HG23	1.84	0.59
1:C:164:TRP:CE3	1:C:165:LEU:HB2	2.37	0.59
1:C:185:ILE:HD13	1:C:708:ILE:CD1	2.33	0.59
1:C:613:TYR:CZ	1:C:617:ILE:HD11	2.37	0.59
1:B:390:PRO:HB2	1:B:412:LEU:HD11	1.85	0.59
1:C:191:ARG:CD	1:C:700:PRO:HB2	2.32	0.58
1:C:414:MET:HG2	1:C:651:LEU:CD1	2.32	0.58
1:D:399:ILE:HD11	1:D:671:LEU:HD21	1.86	0.58
1:A:131:LEU:HD21	1:A:305:ILE:CD1	2.33	0.58
1:A:643:LEU:O	1:A:647:MET:HG2	2.03	0.58
1:B:208:VAL:HG22	1:B:574:VAL:HG13	1.85	0.58
1:C:514:PHE:CE1	1:C:638:LEU:HB3	2.38	0.58
1:D:39:SER:HB2	1:D:103:VAL:CG2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:VAL:O	1:B:494:THR:HG23	2.03	0.58
1:C:86:MET:HE2	1:C:136:PHE:O	2.03	0.58
1:B:25:VAL:CG2	1:B:124:GLN:HG2	2.33	0.58
1:B:216:PRO:HG2	1:B:219:ASP:HB2	1.83	0.58
1:C:57:ILE:HG22	1:C:186:ILE:HG12	1.86	0.58
1:A:491:GLY:HA2	1:A:494:THR:HG22	1.84	0.58
1:A:613:TYR:O	1:A:617:ILE:HG13	2.03	0.58
1:B:141:LEU:HD22	1:B:252:ILE:HG21	1.85	0.58
1:B:480:VAL:HG13	1:B:481:ARG:H	1.68	0.58
1:A:86:MET:HE2	1:A:136:PHE:O	2.03	0.58
1:A:248:PHE:HA	1:A:448:LEU:HD22	1.85	0.58
1:B:54:THR:HA	1:B:57:ILE:HG12	1.85	0.58
1:C:187:ALA:HA	1:C:242:ALA:HB1	1.86	0.58
1:D:122:ALA:HB1	1:D:460:TYR:CD1	2.39	0.58
1:A:102:ASN:OD1	1:A:103:VAL:N	2.36	0.58
1:C:141:LEU:CD2	1:C:252:ILE:HG21	2.34	0.58
1:D:208:VAL:HG11	1:D:577:ILE:HG21	1.84	0.58
1:A:372:SER:O	1:A:376:ILE:HG12	2.03	0.58
1:A:410:LEU:O	1:A:414:MET:HG3	2.04	0.58
1:B:199:LYS:HE2	1:B:696:ASP:HB2	1.85	0.58
1:C:418:PHE:HB3	1:C:419:PRO:HD3	1.85	0.58
1:D:418:PHE:HB3	1:D:419:PRO:HD3	1.85	0.58
1:D:662:ALA:C	1:D:684:LEU:HD21	2.27	0.58
1:B:198:THR:HB	1:B:231:GLY:O	2.03	0.58
1:B:280:LYS:O	1:B:284:GLN:HG3	2.02	0.58
1:B:326:TRP:O	1:B:330:LEU:HD13	2.04	0.58
1:B:580:GLN:O	1:B:584:ILE:HG22	2.04	0.58
1:C:117:PRO:O	1:C:121:VAL:HG23	2.04	0.58
1:D:17:PHE:CD2	1:D:131:LEU:HD11	2.39	0.58
1:D:608:LEU:HD23	1:D:611:MET:CE	2.33	0.58
1:A:6:LEU:HD23	1:A:10:ILE:HD11	1.85	0.57
1:A:141:LEU:HD21	1:A:252:ILE:HG21	1.86	0.57
1:B:569:ALA:HB2	1:B:606:ASN:OD1	2.03	0.57
1:B:663:LYS:HA	1:B:684:LEU:CD2	2.34	0.57
1:C:50:LEU:HD21	1:C:92:ILE:HA	1.85	0.57
1:C:424:LEU:CD1	1:C:507:ILE:HD12	2.34	0.57
1:D:81:LEU:O	1:D:85:VAL:HG23	2.04	0.57
1:A:704:ILE:O	1:A:708:ILE:HG22	2.04	0.57
1:B:317:PRO:O	1:B:321:LEU:HG	2.03	0.57
1:B:410:LEU:O	1:B:414:MET:HG3	2.04	0.57
1:C:41:TYR:CD2	1:C:226:ILE:HD13	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:PHE:O	1:D:252:ILE:HG13	2.04	0.57
1:A:211:THR:HG23	1:A:212:GLU:HG3	1.85	0.57
1:A:448:LEU:HD21	1:A:451:VAL:HB	1.85	0.57
1:B:95:MET:HA	1:B:237:VAL:CG1	2.34	0.57
1:D:50:LEU:HD21	1:D:92:ILE:CG1	2.16	0.57
1:C:327:THR:O	1:C:330:LEU:HG	2.04	0.57
1:C:647:MET:HE2	1:C:647:MET:HA	1.86	0.57
1:D:558:PHE:O	1:D:562:LEU:HD13	2.03	0.57
1:A:97:MET:HE3	1:A:128:VAL:CG2	2.34	0.57
1:A:539:MET:CE	1:B:539:MET:HE3	2.32	0.57
1:C:704:ILE:O	1:C:708:ILE:HG22	2.04	0.57
1:D:50:LEU:HD11	1:D:92:ILE:HA	1.86	0.57
1:A:102:ASN:O	1:A:105:VAL:HG12	2.04	0.57
1:A:210:LYS:HE3	1:A:217:GLU:HB2	1.85	0.57
1:B:226:ILE:HG21	1:B:596:TYR:HB3	1.85	0.57
1:D:283:ILE:O	1:D:287:ILE:HG13	2.04	0.57
1:D:301:SER:HB3	1:D:452:ALA:HB3	1.85	0.57
1:B:129:MET:HE3	1:B:241:GLY:CA	2.34	0.57
1:B:220:PRO:HD3	1:B:472:GLU:O	2.05	0.57
1:B:547:GLY:O	1:B:637:VAL:HA	2.04	0.57
1:B:671:LEU:HD23	1:B:672:GLU:N	2.19	0.57
1:D:265:ILE:HG13	1:D:266:TYR:N	2.19	0.57
1:A:307:TYR:O	1:A:311:LYS:HB2	2.05	0.57
1:B:103:VAL:HG22	1:B:470:ILE:CD1	2.31	0.57
1:B:573:MET:HE3	1:B:573:MET:HA	1.86	0.57
1:D:199:LYS:HD2	1:D:692:ASP:HB3	1.86	0.57
1:D:232:ASP:O	1:D:236:ASP:HB2	2.05	0.57
1:D:401:GLY:O	1:D:405:VAL:HG23	2.04	0.57
1:B:199:LYS:CE	1:B:696:ASP:HB2	2.34	0.57
1:A:197:TYR:OH	1:A:600:ILE:HG23	2.04	0.56
1:B:187:ALA:HA	1:B:242:ALA:HB1	1.87	0.56
1:C:401:GLY:O	1:C:405:VAL:HG23	2.05	0.56
1:D:558:PHE:HE1	1:D:614:PRO:HB2	1.69	0.56
1:A:130:GLY:HA2	1:A:455:VAL:HG23	1.87	0.56
1:B:490:VAL:O	1:B:493:THR:HG22	2.05	0.56
1:C:244:LEU:CD2	1:C:455:VAL:HG22	2.35	0.56
1:C:684:LEU:O	1:C:684:LEU:HD23	2.05	0.56
1:A:205:ALA:HB2	1:A:224:ALA:CB	2.35	0.56
1:A:258:LEU:HD23	1:A:438:TYR:HA	1.88	0.56
1:B:138:LEU:HD12	1:B:298:LEU:HD13	1.87	0.56
1:D:39:SER:CB	1:D:103:VAL:HG21	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ALA:CA	1:D:573:MET:HE1	2.24	0.56
1:D:573:MET:SD	1:D:603:THR:HG22	2.46	0.56
1:C:49:PHE:CE2	1:C:234:VAL:HG21	2.40	0.56
1:C:80:PHE:HA	1:C:178:GLY:O	2.05	0.56
1:C:189:PHE:HE1	1:C:612:GLY:HA2	1.71	0.56
1:D:189:PHE:CE1	1:D:615:ALA:HB3	2.40	0.56
1:D:267:VAL:HG12	1:D:276:HIS:HA	1.87	0.56
1:A:191:ARG:NH1	1:A:700:PRO:HG2	2.20	0.56
1:A:213:LEU:HB3	1:A:215:LEU:HD13	1.86	0.56
1:A:545:ILE:HD13	1:B:511:LEU:HD12	1.86	0.56
1:A:522:ILE:HD11	1:A:534:VAL:HG21	1.86	0.56
1:B:218:ASP:HA	1:B:225:THR:HG22	1.87	0.56
1:C:86:MET:HE3	1:C:136:PHE:HB3	1.87	0.56
1:C:102:ASN:OD1	1:C:103:VAL:N	2.39	0.56
1:C:201:ALA:HA	1:C:573:MET:SD	2.46	0.56
1:C:244:LEU:HD23	1:C:455:VAL:HG22	1.88	0.56
1:C:327:THR:HA	1:C:330:LEU:HD21	1.85	0.56
1:C:337:ALA:HB2	1:C:363:TRP:CE2	2.40	0.56
1:C:550:LEU:O	1:C:554:ILE:HG13	2.05	0.56
1:D:398:SER:HA	1:D:405:VAL:CG2	2.36	0.56
1:A:73:THR:O	1:A:76:THR:HB	2.06	0.56
1:A:77:GLY:O	1:A:81:LEU:HD23	2.06	0.56
1:B:371:PHE:O	1:B:375:LEU:HD23	2.06	0.56
1:C:229:ASN:HD21	1:C:473:MET:HE3	1.71	0.56
1:A:221:ARG:O	1:A:594:PRO:HG2	2.05	0.56
1:A:293:PHE:CE1	1:A:336:THR:HG21	2.41	0.56
1:A:300:CYS:CB	1:A:332:THR:HG1	2.18	0.56
1:A:566:VAL:HG11	1:A:693:PRO:HB3	1.87	0.56
1:B:564:SER:HA	1:B:567:THR:HG22	1.87	0.56
1:C:194:GLY:O	1:C:198:THR:HG22	2.06	0.56
1:B:331:LEU:O	1:B:335:LEU:HD13	2.06	0.56
1:A:143:LEU:O	1:A:147:ILE:HG13	2.06	0.55
1:A:663:LYS:HA	1:A:684:LEU:HD12	1.88	0.55
1:B:256:ILE:HD11	1:B:290:PRO:HG2	1.88	0.55
1:B:613:TYR:O	1:B:617:ILE:HG13	2.06	0.55
1:C:259:ALA:HA	1:C:262:MET:CE	2.15	0.55
1:D:73:THR:O	1:D:76:THR:HB	2.05	0.55
1:A:536:LEU:HD21	1:B:536:LEU:CD1	2.36	0.55
1:B:149:GLY:HA3	1:B:155:VAL:HG23	1.88	0.55
1:B:421:THR:O	1:B:425:VAL:HG23	2.06	0.55
1:B:647:MET:HE2	1:B:647:MET:CA	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:VAL:HG21	1:C:339:LEU:HD22	1.88	0.55
1:D:94:GLY:HA3	1:D:129:MET:SD	2.46	0.55
1:D:127:SER:HB2	1:D:305:ILE:HG21	1.88	0.55
1:A:10:ILE:HG23	1:A:302:MET:HE1	1.87	0.55
1:B:49:PHE:CE2	1:B:234:VAL:HG11	2.41	0.55
1:B:126:GLY:HA2	1:B:459:SER:OG	2.06	0.55
1:B:376:ILE:CD1	1:B:424:LEU:HD21	2.36	0.55
1:C:8:PHE:CD2	1:C:146:LEU:HD11	2.40	0.55
1:C:319:ARG:O	1:C:323:ILE:HG13	2.06	0.55
1:D:193:GLY:HA3	1:D:611:MET:HE2	1.88	0.55
1:D:267:VAL:CG1	1:D:276:HIS:HD2	2.19	0.55
1:D:519:PHE:O	1:D:522:ILE:HG22	2.05	0.55
1:A:262:MET:O	1:A:266:TYR:HD2	1.88	0.55
1:A:522:ILE:HD11	1:A:534:VAL:CG1	2.35	0.55
1:B:414:MET:O	1:B:417:VAL:HG12	2.07	0.55
1:D:31:GLY:N	1:D:107:GLU:HB2	2.19	0.55
1:D:107:GLU:O	1:D:110:ARG:HG3	2.06	0.55
1:A:50:LEU:HD21	1:A:92:ILE:HG12	1.88	0.55
1:A:187:ALA:HA	1:A:242:ALA:HB1	1.88	0.55
1:A:299:GLY:HA2	1:A:302:MET:HE3	1.89	0.55
1:B:372:SER:O	1:B:376:ILE:HG13	2.06	0.55
1:D:414:MET:HA	1:D:651:LEU:HD12	1.87	0.55
1:A:137:ALA:HB2	1:A:245:LEU:HG	1.87	0.55
1:A:308:VAL:HG21	1:A:324:SER:OG	2.06	0.55
1:A:511:LEU:CD1	1:B:545:ILE:HD13	2.36	0.55
1:B:663:LYS:HE2	1:B:688:ASP:OD2	2.06	0.55
1:C:105:VAL:CG2	1:C:467:ALA:HB2	2.37	0.55
1:A:21:ASN:HB3	1:A:128:VAL:HG22	1.88	0.55
1:A:311:LYS:HG2	1:A:312:LYS:N	2.22	0.55
1:A:447:MET:HE1	1:A:508:PHE:HE2	1.71	0.55
1:D:138:LEU:HD12	1:D:295:LEU:HD23	1.87	0.55
1:D:199:LYS:CE	1:D:696:ASP:HB2	2.37	0.55
1:A:200:ALA:CB	1:A:569:ALA:HB3	2.37	0.55
1:C:57:ILE:HG12	1:C:189:PHE:HB3	1.88	0.55
1:D:246:GLU:CD	1:D:707:LYS:HE2	2.32	0.55
1:D:563:ILE:CD1	1:D:693:PRO:HB2	2.37	0.55
1:A:386:TYR:HA	1:A:391:THR:HB	1.89	0.55
1:B:162:THR:HA	1:B:167:ILE:O	2.07	0.55
1:B:517:TYR:HB2	1:B:714:VAL:HG22	1.88	0.55
1:D:301:SER:O	1:D:305:ILE:HG13	2.06	0.55
1:A:131:LEU:HD21	1:A:305:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD22	1:A:455:VAL:HG12	1.89	0.55
1:B:666:LEU:HD23	1:B:681:HIS:HA	1.90	0.55
1:C:248:PHE:O	1:C:252:ILE:HG13	2.07	0.55
1:C:293:PHE:CE1	1:C:336:THR:HG21	2.42	0.55
1:C:399:ILE:HD11	1:C:671:LEU:HD21	1.89	0.55
1:B:28:LYS:HA	1:B:104:ARG:CB	2.37	0.54
1:B:299:GLY:HA2	1:B:302:MET:CE	2.36	0.54
1:C:280:LYS:O	1:C:284:GLN:HG3	2.08	0.54
1:A:335:LEU:HD23	1:A:335:LEU:O	2.08	0.54
1:B:22:PHE:O	1:B:26:VAL:HB	2.08	0.54
1:C:8:PHE:O	1:C:11:PRO:HD2	2.07	0.54
1:C:172:PHE:O	1:C:176:VAL:HG22	2.07	0.54
1:C:205:ALA:HB2	1:C:224:ALA:CB	2.37	0.54
1:A:119:LEU:HD13	1:A:317:PRO:CB	2.35	0.54
1:A:220:PRO:O	1:A:596:TYR:OH	2.21	0.54
1:B:15:LEU:HD11	1:B:136:PHE:CE1	2.42	0.54
1:B:140:GLY:HA3	1:B:179:TYR:OH	2.08	0.54
1:B:350:LEU:O	1:B:355:PHE:HB2	2.06	0.54
1:B:401:GLY:O	1:B:405:VAL:HG23	2.08	0.54
1:C:216:PRO:HG2	1:C:219:ASP:HB2	1.88	0.54
1:C:329:ALA:O	1:C:333:VAL:HG23	2.07	0.54
1:C:554:ILE:HG12	1:D:418:PHE:HE2	1.73	0.54
1:C:643:LEU:O	1:C:647:MET:HG2	2.08	0.54
1:B:130:GLY:HA2	1:B:455:VAL:HB	1.89	0.54
1:C:47:ASP:OD1	1:C:95:MET:HE1	2.08	0.54
1:C:652:THR:HB	1:C:694:LEU:O	2.07	0.54
1:D:503:ILE:HG12	1:D:649:ALA:CB	2.37	0.54
1:A:172:PHE:O	1:A:176:VAL:HG12	2.08	0.54
1:A:459:SER:C	1:A:462:PRO:HD2	2.32	0.54
1:C:660:ASP:O	1:C:664:LYS:HG3	2.07	0.54
1:D:621:THR:HB	1:D:622:PRO:HD3	1.89	0.54
1:A:246:GLU:OE2	1:A:707:LYS:HE2	2.08	0.54
1:A:596:TYR:O	1:A:600:ILE:HG12	2.07	0.54
1:B:49:PHE:HD2	1:B:234:VAL:HG11	1.69	0.54
1:C:599:CYS:O	1:C:603:THR:HG22	2.07	0.54
1:D:266:TYR:HD1	1:D:531:PRO:CG	2.13	0.54
1:D:364:PHE:O	1:D:368:ILE:HG12	2.08	0.54
1:D:507:ILE:HD11	1:D:646:ALA:HB1	1.88	0.54
1:D:598:ARG:O	1:D:602:ILE:HG13	2.07	0.54
1:B:82:LEU:HD23	1:B:144:VAL:CG2	2.38	0.54
1:B:148:PHE:HB3	1:B:154:GLN:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:LEU:O	1:B:554:ILE:HG12	2.08	0.54
1:C:205:ALA:HB1	1:C:222:ASN:HD21	1.72	0.54
1:D:138:LEU:O	1:D:142:VAL:HG12	2.08	0.54
1:A:49:PHE:HD2	1:A:234:VAL:HG11	1.73	0.54
1:A:130:GLY:CA	1:A:455:VAL:HG23	2.37	0.54
1:B:222:ASN:HB3	1:B:225:THR:HG23	1.90	0.54
1:C:489:ALA:HA	1:C:664:LYS:HE2	1.90	0.54
1:D:199:LYS:HE2	1:D:696:ASP:HB2	1.90	0.54
1:A:6:LEU:CD2	1:A:10:ILE:HD11	2.38	0.54
1:A:491:GLY:O	1:A:494:THR:HG22	2.07	0.54
1:A:578:ARG:NH1	1:B:399:ILE:O	2.41	0.54
1:A:685:VAL:O	1:A:689:THR:HG23	2.08	0.54
1:B:573:MET:O	1:B:577:ILE:HG13	2.08	0.54
1:B:662:ALA:O	1:B:684:LEU:HD21	2.08	0.54
1:D:226:ILE:HG21	1:D:596:TYR:CB	2.35	0.54
1:D:266:TYR:HE2	1:D:352:VAL:HB	1.73	0.54
1:D:507:ILE:HD11	1:D:646:ALA:CB	2.38	0.54
1:A:307:TYR:CZ	1:A:311:LYS:HG3	2.43	0.54
1:B:65:ALA:HB1	1:B:81:LEU:HD21	1.89	0.54
1:B:232:ASP:HB2	1:B:466:ASN:HD21	1.72	0.53
1:A:507:ILE:CD1	1:A:646:ALA:HB2	2.31	0.53
1:B:252:ILE:HD11	1:B:294:ALA:HB2	1.89	0.53
1:D:252:ILE:O	1:D:256:ILE:HG13	2.08	0.53
1:A:149:GLY:CA	1:A:155:VAL:HG13	2.37	0.53
1:A:191:ARG:HH21	1:A:240:LEU:CA	2.21	0.53
1:A:240:LEU:HD21	1:A:458:ASP:CB	2.26	0.53
1:B:39:SER:O	1:B:43:ARG:HG3	2.07	0.53
1:B:259:ALA:HA	1:B:262:MET:HE2	1.91	0.53
1:C:548:ALA:HA	1:C:636:GLY:O	2.08	0.53
1:A:305:ILE:O	1:A:309:ILE:HG23	2.08	0.53
1:A:344:LEU:HA	1:A:347:LEU:CD1	2.38	0.53
1:A:539:MET:SD	1:A:544:VAL:HG12	2.49	0.53
1:B:102:ASN:OD1	1:B:103:VAL:HG23	2.08	0.53
1:D:5:ALA:O	1:D:9:LEU:HD13	2.08	0.53
1:D:53:GLU:O	1:D:57:ILE:HG23	2.09	0.53
1:A:162:THR:HA	1:A:167:ILE:O	2.09	0.53
1:B:7:PHE:O	1:B:295:LEU:HD13	2.09	0.53
1:B:169:PHE:HB2	1:B:174:MET:CG	2.39	0.53
1:C:199:LYS:HG3	1:C:693:PRO:HA	1.90	0.53
1:A:563:ILE:CG2	1:B:411:SER:HB2	2.38	0.53
1:C:57:ILE:HD11	1:C:611:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:MET:O	1:C:266:TYR:HD2	1.91	0.53
1:C:615:ALA:O	1:C:619:ILE:HG13	2.08	0.53
1:D:243:ASP:HA	1:D:704:ILE:HD11	1.89	0.53
1:A:448:LEU:HD23	1:A:451:VAL:HB	1.91	0.53
1:A:514:PHE:CE1	1:A:638:LEU:HB3	2.44	0.53
1:B:98:ALA:HB3	1:B:237:VAL:HG11	1.91	0.53
1:A:84:ALA:HA	1:A:186:ILE:HG13	1.89	0.53
1:A:7:PHE:HA	1:A:10:ILE:HG12	1.89	0.53
1:A:62:ILE:O	1:A:66:ILE:HG12	2.09	0.53
1:B:471:SER:OG	1:B:481:ARG:HB2	2.09	0.53
1:A:53:GLU:OE1	1:A:190:ASP:HA	2.09	0.53
1:A:517:TYR:OH	1:A:631:ALA:O	2.26	0.53
1:B:514:PHE:CE1	1:B:638:LEU:HB3	2.43	0.53
1:B:547:GLY:HA2	1:B:633:PHE:CE1	2.43	0.53
1:C:105:VAL:HG23	1:C:467:ALA:CB	2.38	0.53
1:C:563:ILE:HG22	1:D:411:SER:HB2	1.91	0.53
1:D:172:PHE:O	1:D:176:VAL:HG22	2.09	0.53
1:D:202:ASP:OD2	2:D:801:ZOL:O10	2.27	0.52
1:A:84:ALA:CA	1:A:186:ILE:HG13	2.39	0.52
1:A:253:VAL:HG13	1:A:257:ILE:CD1	2.40	0.52
1:B:9:LEU:HD12	1:B:12:LEU:HD12	1.91	0.52
1:C:170:VAL:HG13	1:C:171:PRO:HD2	1.91	0.52
1:D:43:ARG:CG	1:D:99:THR:HB	2.37	0.52
1:D:548:ALA:HA	1:D:636:GLY:O	2.09	0.52
1:A:288:SER:HB3	1:A:292:PHE:CE2	2.45	0.52
1:B:6:LEU:O	1:B:10:ILE:HG13	2.10	0.52
1:B:194:GLY:O	1:B:198:THR:HG22	2.08	0.52
1:B:493:THR:O	1:B:497:ILE:HG23	2.08	0.52
1:D:620:LEU:O	1:D:624:VAL:HG23	2.09	0.52
1:A:141:LEU:CD2	1:A:252:ILE:HG21	2.40	0.52
1:B:227:ALA:HB2	1:B:600:ILE:HD13	1.91	0.52
1:B:265:ILE:HD12	1:B:522:ILE:HG21	1.92	0.52
1:C:185:ILE:HD12	1:C:619:ILE:CD1	2.34	0.52
1:D:54:THR:HA	1:D:57:ILE:CG1	2.40	0.52
1:A:57:ILE:CD1	1:A:189:PHE:HB3	2.39	0.52
1:A:320:GLU:O	1:A:323:ILE:HG22	2.10	0.52
1:C:331:LEU:HD23	1:C:335:LEU:HD13	1.90	0.52
1:D:54:THR:HA	1:D:57:ILE:CD1	2.38	0.52
1:D:205:ALA:HB2	1:D:224:ALA:CB	2.39	0.52
1:A:647:MET:HE1	1:B:553:ALA:CA	2.38	0.52
1:B:283:ILE:O	1:B:287:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ASN:HA	1:C:600:ILE:CG1	2.40	0.52
1:D:30:GLU:HA	1:D:107:GLU:CD	2.35	0.52
1:D:388:TYR:O	1:D:392:GLN:HG3	2.10	0.52
1:A:620:LEU:O	1:A:624:VAL:HG22	2.10	0.52
1:C:205:ALA:HB2	1:C:224:ALA:HB3	1.90	0.52
1:D:390:PRO:HB2	1:D:412:LEU:HD11	1.92	0.52
1:B:363:TRP:CE2	1:B:367:ILE:HD11	2.44	0.52
1:B:413:GLY:HA3	1:B:655:SER:HB2	1.92	0.52
1:B:707:LYS:O	1:B:711:VAL:HG23	2.10	0.52
1:D:519:PHE:CE1	1:D:535:LEU:HD21	2.45	0.52
1:A:211:THR:CG2	1:A:212:GLU:HG3	2.40	0.52
1:A:253:VAL:O	1:A:257:ILE:HD12	2.10	0.52
1:A:503:ILE:HD12	1:A:649:ALA:CB	2.29	0.52
1:B:25:VAL:HG21	1:B:124:GLN:HG2	1.91	0.52
1:B:97:MET:CE	1:B:125:GLY:HA2	2.40	0.52
1:C:522:ILE:HD11	1:C:534:VAL:CG1	2.33	0.52
1:D:104:ARG:O	1:D:107:GLU:HG2	2.10	0.52
1:A:711:VAL:O	1:A:714:VAL:HG12	2.10	0.51
1:B:25:VAL:HG21	1:B:97:MET:HE1	1.93	0.51
1:C:325:LEU:HD13	1:C:453:THR:CG2	2.40	0.51
1:A:296:VAL:CG1	1:A:335:LEU:HD22	2.40	0.51
1:C:199:LYS:CE	1:C:696:ASP:HB2	2.38	0.51
1:D:276:HIS:O	1:D:277:GLN:HB2	2.09	0.51
1:D:480:VAL:O	1:D:484:THR:HG23	2.09	0.51
1:B:286:LEU:HD21	1:B:355:PHE:HE2	1.75	0.51
1:C:398:SER:HA	1:C:405:VAL:CG2	2.39	0.51
1:D:267:VAL:HG12	1:D:276:HIS:HD2	1.76	0.51
1:D:588:LEU:HD23	1:D:588:LEU:H	1.75	0.51
1:B:162:THR:HG23	1:B:162:THR:O	2.09	0.51
1:C:149:GLY:HA3	1:C:155:VAL:HG23	1.93	0.51
1:C:613:TYR:O	1:C:617:ILE:HG13	2.10	0.51
1:A:21:ASN:OD1	1:A:124:GLN:HB3	2.10	0.51
1:B:414:MET:HG2	1:B:651:LEU:CD1	2.36	0.51
1:C:102:ASN:O	1:C:105:VAL:HG22	2.10	0.51
1:C:129:MET:HE3	1:C:133:VAL:CG2	2.39	0.51
1:C:666:LEU:HD23	1:C:666:LEU:O	2.10	0.51
1:B:308:VAL:HG21	1:B:324:SER:CB	2.38	0.51
1:C:84:ALA:O	1:C:186:ILE:HD12	2.11	0.51
1:C:521:GLN:HG2	1:C:717:VAL:CG2	2.39	0.51
1:D:182:GLY:O	1:D:185:ILE:HG22	2.10	0.51
1:B:102:ASN:O	1:B:105:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:GLU:O	1:C:57:ILE:HG13	2.11	0.51
1:C:233:ASN:O	1:C:237:VAL:HB	2.10	0.51
1:C:537:LEU:HD23	1:C:639:ILE:HD11	1.92	0.51
1:D:218:ASP:HA	1:D:225:THR:CG2	2.40	0.51
1:A:543:ARG:NH1	1:A:629:LEU:O	2.43	0.51
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.92	0.51
1:C:185:ILE:CD1	1:C:708:ILE:HD11	2.40	0.51
1:D:23:ALA:HA	1:D:26:VAL:HG12	1.93	0.51
1:D:104:ARG:HA	1:D:107:GLU:CD	2.36	0.51
1:D:451:VAL:O	1:D:455:VAL:HG23	2.10	0.51
1:D:643:LEU:O	1:D:647:MET:HG2	2.11	0.51
1:A:666:LEU:HD23	1:A:666:LEU:O	2.11	0.51
1:B:563:ILE:HG13	1:B:698:VAL:HG21	1.93	0.51
1:C:141:LEU:HD21	1:C:252:ILE:CG2	2.41	0.51
1:C:331:LEU:O	1:C:335:LEU:HD13	2.10	0.51
1:B:11:PRO:O	1:B:15:LEU:HD23	2.10	0.51
1:D:170:VAL:HG13	1:D:171:PRO:HD2	1.93	0.51
1:A:247:SER:HA	1:A:707:LYS:HE3	1.92	0.50
1:A:707:LYS:O	1:A:711:VAL:HG23	2.11	0.50
1:B:75:GLN:HA	1:B:78:VAL:CG1	2.39	0.50
1:B:75:GLN:CA	1:B:78:VAL:HG12	2.40	0.50
1:B:160:ILE:HD11	1:B:527:ILE:HD12	1.93	0.50
1:C:115:ILE:HG12	1:C:483:ILE:HG23	1.93	0.50
1:D:123:TYR:CE2	1:D:305:ILE:HG23	2.46	0.50
1:A:200:ALA:HB2	1:A:569:ALA:HB3	1.92	0.50
1:C:259:ALA:CA	1:C:262:MET:HE2	2.16	0.50
1:D:147:ILE:HG13	1:D:148:PHE:CD2	2.45	0.50
1:D:188:MET:HG2	1:D:615:ALA:HB2	1.92	0.50
1:A:54:THR:HG23	1:A:58:PHE:CE2	2.46	0.50
1:A:97:MET:SD	1:A:125:GLY:HA2	2.51	0.50
1:B:159:ASN:HB2	1:B:161:TYR:CE1	2.44	0.50
1:B:459:SER:C	1:B:462:PRO:HD2	2.37	0.50
1:C:404:MET:HE2	1:D:571:MET:N	2.26	0.50
1:D:38:ILE:HD12	1:D:38:ILE:H	1.76	0.50
1:D:73:THR:HG22	1:D:75:GLN:H	1.76	0.50
1:D:184:SER:CB	1:D:246:GLU:HG3	2.41	0.50
1:A:65:ALA:HB2	1:A:81:LEU:HD21	1.94	0.50
1:A:561:TYR:HA	1:B:415:LYS:CE	2.42	0.50
1:B:50:LEU:CD2	1:B:92:ILE:HG13	2.30	0.50
1:B:138:LEU:O	1:B:142:VAL:HG12	2.11	0.50
1:C:364:PHE:O	1:C:368:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:MET:SD	1:C:544:VAL:HG12	2.51	0.50
1:C:571:MET:HG2	1:D:400:GLU:HG3	1.94	0.50
1:D:187:ALA:HA	1:D:242:ALA:HB1	1.93	0.50
1:D:569:ALA:HB2	1:D:606:ASN:ND2	2.26	0.50
1:B:95:MET:HA	1:B:237:VAL:HG12	1.93	0.50
1:C:597:ASN:HA	1:C:600:ILE:CD1	2.41	0.50
1:D:210:LYS:NZ	1:D:217:GLU:HB2	2.27	0.50
1:D:266:TYR:HA	1:D:531:PRO:HG2	1.92	0.50
1:D:550:LEU:O	1:D:554:ILE:HG13	2.11	0.50
1:A:248:PHE:O	1:A:252:ILE:HG13	2.12	0.50
1:A:465:ASP:OD1	5:A:902:HOH:O	2.20	0.50
1:B:54:THR:O	1:B:57:ILE:HG12	2.12	0.50
1:B:663:LYS:O	1:B:667:GLU:HG3	2.10	0.50
1:C:306:LEU:O	1:C:309:ILE:HG12	2.11	0.50
1:C:618:ALA:HB2	1:C:705:LEU:HD12	1.93	0.50
1:D:414:MET:HG2	1:D:651:LEU:CD1	2.38	0.50
1:A:65:ALA:HB1	1:A:81:LEU:HD21	1.93	0.50
1:B:75:GLN:C	1:B:78:VAL:HG12	2.36	0.50
1:B:124:GLN:O	1:B:128:VAL:HG23	2.12	0.50
1:B:353:LEU:HD11	1:B:355:PHE:CG	2.47	0.50
1:B:682:LYS:O	1:B:686:ILE:HG12	2.11	0.50
1:D:127:SER:O	1:D:131:LEU:HG	2.12	0.50
1:D:167:ILE:HG12	1:D:719:ILE:HG12	1.94	0.50
1:D:386:TYR:HA	1:D:391:THR:HB	1.94	0.50
1:A:32:THR:HG22	1:A:34:ARG:H	1.77	0.50
1:C:25:VAL:HB	1:C:97:MET:HE1	1.93	0.50
1:C:647:MET:HE2	1:C:647:MET:CA	2.42	0.50
1:A:622:PRO:HG3	1:A:709:MET:CG	2.34	0.50
1:A:686:ILE:O	1:A:690:VAL:HG23	2.12	0.50
1:D:31:GLY:H	1:D:107:GLU:CB	2.21	0.50
1:D:58:PHE:O	1:D:62:ILE:HG13	2.12	0.50
1:A:97:MET:HE3	1:A:128:VAL:HB	1.93	0.49
1:B:573:MET:SD	1:B:599:CYS:HB3	2.52	0.49
1:D:363:TRP:CE2	1:D:367:ILE:HD11	2.47	0.49
1:A:288:SER:HB2	1:A:343:TYR:OH	2.11	0.49
1:C:308:VAL:HG22	1:C:324:SER:CB	2.42	0.49
1:D:124:GLN:O	1:D:128:VAL:HG13	2.11	0.49
1:B:7:PHE:HB3	1:B:295:LEU:HD13	1.93	0.49
1:B:293:PHE:HD2	1:B:445:LEU:HD23	1.76	0.49
1:C:666:LEU:HD13	1:C:681:HIS:HA	1.93	0.49
1:A:65:ALA:CB	1:A:81:LEU:CD2	2.88	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ILE:HG23	1:B:487:LEU:HD21	1.93	0.49
1:A:14:ALA:HB2	1:A:302:MET:SD	2.52	0.49
1:A:258:LEU:O	1:A:262:MET:HG3	2.12	0.49
1:A:344:LEU:HA	1:A:347:LEU:HD12	1.93	0.49
1:A:375:LEU:HB2	1:A:423:THR:HG21	1.94	0.49
1:B:220:PRO:HA	1:B:473:MET:SD	2.53	0.49
1:B:256:ILE:CD1	1:B:290:PRO:HG2	2.42	0.49
1:D:184:SER:OG	1:D:708:ILE:CG2	2.60	0.49
1:B:138:LEU:HD21	1:B:294:ALA:HB1	1.94	0.49
1:C:389:LYS:N	1:C:390:PRO:HD2	2.28	0.49
1:D:185:ILE:HD11	1:D:615:ALA:HB1	1.93	0.49
1:D:208:VAL:HA	1:D:212:GLU:CD	2.38	0.49
1:C:60:VAL:O	1:C:64:ILE:HG13	2.13	0.49
1:A:220:PRO:CD	1:A:473:MET:HA	2.42	0.49
1:B:25:VAL:HG23	1:B:97:MET:HE1	1.94	0.49
1:C:623:LEU:HD12	1:C:627:PHE:HE2	1.78	0.49
1:C:663:LYS:HB2	1:C:684:LEU:CD2	2.43	0.49
1:D:453:THR:O	1:D:456:SER:OG	2.22	0.49
1:D:647:MET:HE2	1:D:647:MET:CA	2.42	0.49
1:A:185:ILE:CD1	1:A:708:ILE:HD11	2.43	0.49
1:A:466:ASN:O	1:A:470:ILE:HG13	2.13	0.49
1:B:97:MET:HE3	1:B:125:GLY:HA2	1.95	0.49
1:A:54:THR:HG23	1:A:58:PHE:CD2	2.48	0.48
1:A:500:GLY:O	1:A:503:ILE:HG22	2.12	0.48
1:B:240:LEU:HD21	1:B:458:ASP:HB3	1.94	0.48
1:B:286:LEU:CD1	1:B:353:LEU:HD22	2.43	0.48
1:C:41:TYR:HD2	1:C:226:ILE:HD13	1.76	0.48
1:D:301:SER:CB	1:D:452:ALA:HB3	2.42	0.48
1:D:355:PHE:CE1	1:D:362:PRO:HD3	2.47	0.48
1:A:40:SER:HA	1:A:43:ARG:HG2	1.94	0.48
1:A:569:ALA:HB2	1:A:606:ASN:OD1	2.12	0.48
1:B:664:LYS:HD2	2:B:801:ZOL:N17	2.27	0.48
1:C:34:ARG:O	1:C:38:ILE:HG12	2.13	0.48
1:C:539:MET:HG2	1:D:539:MET:HE1	1.94	0.48
1:D:191:ARG:NH1	1:D:700:PRO:HG2	2.27	0.48
1:A:8:PHE:O	1:A:11:PRO:HD2	2.12	0.48
1:A:103:VAL:HG12	1:A:470:ILE:HD13	1.94	0.48
1:A:141:LEU:HD21	1:A:252:ILE:CG2	2.42	0.48
1:A:394:LEU:HD21	1:A:659:TRP:CD1	2.48	0.48
1:A:518:MET:SD	1:A:521:GLN:NE2	2.86	0.48
1:B:587:LEU:HD11	1:B:594:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:656:GLY:HA3	1:C:695:LYS:HB3	1.96	0.48
1:A:519:PHE:HD1	1:A:534:VAL:HG11	1.77	0.48
1:B:90:ALA:HB2	1:B:136:PHE:HD2	1.77	0.48
1:B:564:SER:O	1:B:567:THR:HG22	2.13	0.48
1:B:88:ALA:O	1:B:92:ILE:HD12	2.14	0.48
1:B:628:LEU:O	1:B:726:PHE:HB2	2.13	0.48
1:C:361:SER:N	1:C:362:PRO:HD2	2.28	0.48
1:A:549:LEU:HD23	1:B:643:LEU:CD2	2.43	0.48
1:A:613:TYR:N	1:A:614:PRO:HD2	2.28	0.48
1:B:223:PRO:HA	1:B:596:TYR:CE2	2.48	0.48
1:C:219:ASP:OD2	1:C:221:ARG:HB2	2.14	0.48
1:A:266:TYR:CE1	1:A:531:PRO:HG2	2.49	0.48
1:B:80:PHE:CE2	1:B:182:GLY:HA2	2.48	0.48
1:B:480:VAL:O	1:B:484:THR:HG23	2.13	0.48
1:C:244:LEU:HD23	1:C:455:VAL:CG2	2.44	0.48
1:C:457:VAL:HG13	1:C:460:TYR:HE1	1.79	0.48
1:C:518:MET:SD	1:C:521:GLN:NE2	2.87	0.48
1:D:227:ALA:HA	1:D:230:VAL:HG12	1.96	0.48
1:B:170:VAL:HG13	1:B:171:PRO:HD2	1.95	0.48
1:B:389:LYS:N	1:B:390:PRO:HD2	2.29	0.48
1:C:344:LEU:HD22	1:C:347:LEU:HD12	1.95	0.48
1:C:623:LEU:O	1:C:627:PHE:HD2	1.96	0.48
1:C:710:SER:O	1:C:714:VAL:HG23	2.14	0.48
1:D:189:PHE:CZ	1:D:615:ALA:HB3	2.48	0.48
1:D:205:ALA:HB2	1:D:224:ALA:HB3	1.95	0.48
1:A:126:GLY:O	1:A:456:SER:HA	2.14	0.48
1:A:133:VAL:HG13	1:A:245:LEU:HB2	1.96	0.48
1:B:185:ILE:CD1	1:B:708:ILE:HD11	2.40	0.48
1:B:364:PHE:O	1:B:368:ILE:HG12	2.14	0.48
1:C:58:PHE:O	1:C:62:ILE:HG13	2.13	0.48
1:C:404:MET:HE2	1:D:571:MET:CA	2.43	0.48
1:D:376:ILE:HD11	1:D:424:LEU:CD2	2.44	0.48
1:D:613:TYR:N	1:D:614:PRO:HD2	2.28	0.48
1:A:138:LEU:O	1:A:142:VAL:HG12	2.13	0.48
1:A:263:PHE:HB3	1:A:264:PRO:HD3	1.95	0.48
1:B:99:THR:HG22	1:B:233:ASN:ND2	2.28	0.48
1:C:425:VAL:HG21	1:D:550:LEU:HD23	1.94	0.48
1:D:8:PHE:O	1:D:11:PRO:HD2	2.14	0.48
1:D:147:ILE:HD11	1:D:148:PHE:CE2	2.49	0.48
1:A:226:ILE:HG22	1:A:596:TYR:HB3	1.94	0.47
1:A:285:ALA:O	1:A:343:TYR:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PRO:HA	1:B:596:TYR:CD2	2.49	0.47
1:B:633:PHE:O	1:B:637:VAL:HG23	2.14	0.47
1:A:244:LEU:HD23	1:A:455:VAL:CG1	2.45	0.47
1:A:506:ALA:HB2	1:A:707:LYS:HZ2	1.78	0.47
1:A:521:GLN:HG2	1:A:717:VAL:CG2	2.43	0.47
1:C:191:ARG:HH21	1:C:240:LEU:CA	2.26	0.47
1:C:202:ASP:OD1	1:C:202:ASP:C	2.57	0.47
1:A:681:HIS:O	1:A:685:VAL:HG23	2.15	0.47
1:B:43:ARG:HG2	1:B:99:THR:HB	1.96	0.47
1:B:198:THR:HB	1:B:231:GLY:C	2.39	0.47
1:B:298:LEU:HD23	1:B:302:MET:HE2	1.97	0.47
1:B:576:GLU:OE2	1:B:598:ARG:HD3	2.15	0.47
1:D:268:GLN:O	1:D:275:VAL:HG22	2.14	0.47
1:A:58:PHE:O	1:A:62:ILE:HG13	2.14	0.47
1:A:307:TYR:O	1:A:311:LYS:N	2.47	0.47
1:A:320:GLU:HA	1:A:323:ILE:HG22	1.95	0.47
1:A:556:TYR:CE2	1:B:647:MET:HB3	2.48	0.47
1:B:25:VAL:HG11	1:B:124:GLN:CB	2.45	0.47
1:B:58:PHE:O	1:B:62:ILE:HG13	2.15	0.47
1:B:288:SER:HB2	1:B:292:PHE:HE2	1.79	0.47
1:B:709:MET:HE3	1:B:709:MET:HB2	1.81	0.47
1:C:480:VAL:O	1:C:484:THR:HG23	2.15	0.47
1:D:492:ASN:OD1	1:D:493:THR:HG23	2.14	0.47
1:D:633:PHE:O	1:D:637:VAL:HG23	2.15	0.47
1:A:6:LEU:O	1:A:10:ILE:HG12	2.14	0.47
1:A:288:SER:HB3	1:A:292:PHE:CZ	2.50	0.47
1:C:54:THR:HG23	1:C:58:PHE:CD2	2.49	0.47
1:D:10:ILE:CG2	1:D:298:LEU:HD22	2.45	0.47
1:D:126:GLY:O	1:D:456:SER:HA	2.15	0.47
1:D:218:ASP:HA	1:D:225:THR:HG22	1.95	0.47
1:A:93:VAL:HG11	1:A:132:SER:OG	2.14	0.47
1:A:110:ARG:HG3	1:A:480:VAL:HG11	1.97	0.47
1:A:633:PHE:O	1:A:637:VAL:HG23	2.15	0.47
1:B:110:ARG:HD2	1:B:110:ARG:C	2.39	0.47
1:B:194:GLY:HA3	1:B:235:GLY:HA2	1.95	0.47
1:B:286:LEU:HD11	1:B:353:LEU:HD22	1.95	0.47
1:B:304:GLY:O	1:B:308:VAL:HG23	2.14	0.47
1:B:317:PRO:HG2	1:B:486:HIS:CE1	2.50	0.47
1:B:573:MET:HE3	1:B:573:MET:O	2.14	0.47
1:C:18:ALA:HB2	1:C:131:LEU:CB	2.44	0.47
1:D:54:THR:HA	1:D:57:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:CG1	1:D:467:ALA:HB2	2.44	0.47
1:D:244:LEU:HD23	1:D:455:VAL:CG2	2.43	0.47
1:D:419:PRO:N	1:D:420:PRO:HD2	2.30	0.47
1:A:323:ILE:O	1:A:327:THR:HG23	2.14	0.47
1:A:651:LEU:HD23	1:A:651:LEU:C	2.40	0.47
1:B:7:PHE:HB3	1:B:295:LEU:CD1	2.45	0.47
1:B:286:LEU:HD11	1:B:353:LEU:CD2	2.45	0.47
1:C:248:PHE:CZ	1:C:294:ALA:HB1	2.50	0.47
1:C:622:PRO:HG3	1:C:709:MET:CG	2.43	0.47
1:A:711:VAL:HA	1:A:714:VAL:HG12	1.97	0.47
1:C:199:LYS:HG3	1:C:697:THR:HG23	1.97	0.47
1:A:506:ALA:HB2	1:A:707:LYS:NZ	2.30	0.47
1:A:543:ARG:HH22	1:A:726:PHE:C	2.23	0.47
1:A:588:LEU:HD12	1:A:588:LEU:H	1.78	0.47
1:B:105:VAL:HG23	1:B:121:VAL:HB	1.96	0.47
1:C:283:ILE:O	1:C:287:ILE:HG13	2.15	0.47
1:C:370:ILE:HG12	1:C:446:GLY:O	2.15	0.47
1:A:189:PHE:HE1	1:A:612:GLY:HA2	1.80	0.46
1:C:138:LEU:O	1:C:142:VAL:HG12	2.15	0.46
1:D:80:PHE:CE2	1:D:182:GLY:HA2	2.50	0.46
1:D:184:SER:CB	1:D:708:ILE:HG22	2.44	0.46
1:A:130:GLY:HA2	1:A:455:VAL:HG21	1.96	0.46
1:A:400:GLU:HG3	1:B:571:MET:HE3	1.97	0.46
1:C:176:VAL:HB	1:C:253:VAL:HG13	1.96	0.46
1:C:300:CYS:HB2	1:C:332:THR:OG1	2.16	0.46
1:C:444:ALA:HB2	1:C:508:PHE:HB2	1.94	0.46
1:A:248:PHE:CZ	1:A:252:ILE:HD11	2.50	0.46
1:B:227:ALA:HB2	1:B:600:ILE:CD1	2.45	0.46
1:D:189:PHE:HE1	1:D:612:GLY:HA2	1.81	0.46
1:D:377:GLY:HA2	1:D:497:ILE:HG12	1.98	0.46
1:B:651:LEU:C	1:B:651:LEU:HD23	2.41	0.46
1:C:86:MET:HE3	1:C:136:PHE:CB	2.45	0.46
1:C:191:ARG:HD3	1:C:700:PRO:CB	2.35	0.46
1:C:200:ALA:CB	1:C:569:ALA:HB3	2.45	0.46
1:D:54:THR:CA	1:D:57:ILE:HG12	2.46	0.46
1:D:361:SER:N	1:D:362:PRO:HD2	2.30	0.46
1:A:18:ALA:O	1:A:128:VAL:HG22	2.15	0.46
1:A:632:GLU:CD	1:A:632:GLU:H	2.23	0.46
1:B:189:PHE:HE1	1:B:612:GLY:HA2	1.80	0.46
1:B:212:GLU:OE2	1:B:578:ARG:NH1	2.46	0.46
1:B:361:SER:N	1:B:362:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ILE:HG23	1:C:364:PHE:HE2	1.80	0.46
1:A:556:TYR:HB3	1:B:417:VAL:HG11	1.98	0.46
1:A:567:THR:HA	1:B:404:MET:HE1	1.98	0.46
1:B:321:LEU:HD22	1:B:457:VAL:HG22	1.98	0.46
1:B:613:TYR:N	1:B:614:PRO:HD2	2.31	0.46
1:C:138:LEU:HD12	1:C:298:LEU:HD22	1.96	0.46
1:A:129:MET:CE	1:A:241:GLY:HA3	2.46	0.46
1:A:169:PHE:HB2	1:A:174:MET:CG	2.46	0.46
1:A:185:ILE:HD13	1:A:708:ILE:CD1	2.45	0.46
1:A:283:ILE:O	1:A:287:ILE:HG13	2.15	0.46
1:A:425:VAL:HG21	1:B:550:LEU:HB2	1.98	0.46
1:B:210:LYS:HE2	1:B:217:GLU:HB2	1.97	0.46
1:B:323:ILE:O	1:B:327:THR:HG23	2.15	0.46
1:B:366:ALA:O	1:B:370:ILE:HG13	2.16	0.46
1:B:573:MET:HE3	1:B:576:GLU:HB3	1.97	0.46
1:C:383:TYR:HE2	1:C:419:PRO:HG2	1.79	0.46
1:C:623:LEU:O	1:C:627:PHE:CD2	2.69	0.46
1:D:288:SER:HB2	1:D:292:PHE:CE2	2.50	0.46
1:A:245:LEU:HD23	1:A:245:LEU:C	2.40	0.46
1:B:226:ILE:CG2	1:B:596:TYR:HB3	2.45	0.46
1:C:557:TYR:HD1	1:D:415:LYS:HA	1.80	0.46
1:D:622:PRO:HB2	1:D:712:VAL:HG12	1.97	0.46
1:A:53:GLU:HG2	1:A:57:ILE:HD11	1.98	0.46
1:A:191:ARG:HH21	1:A:240:LEU:HA	1.81	0.46
1:A:199:LYS:HE2	1:A:696:ASP:HB2	1.95	0.46
1:A:573:MET:HE2	1:A:599:CYS:O	2.16	0.46
1:B:26:VAL:O	1:B:26:VAL:HG22	2.16	0.46
1:B:95:MET:HB2	1:B:238:ALA:HB2	1.98	0.46
1:B:208:VAL:CG2	1:B:574:VAL:HG13	2.46	0.46
1:B:419:PRO:CB	1:B:420:PRO:HD3	2.46	0.46
1:C:663:LYS:CB	1:C:684:LEU:HD22	2.45	0.46
1:A:556:TYR:CB	1:B:417:VAL:HG11	2.45	0.46
1:B:110:ARG:HG3	1:B:476:LEU:CD2	2.46	0.46
1:C:208:VAL:HG23	1:C:574:VAL:HG22	1.97	0.46
1:D:226:ILE:O	1:D:230:VAL:HG12	2.16	0.46
1:D:489:ALA:HA	1:D:492:ASN:ND2	2.30	0.46
1:A:491:GLY:HA2	1:A:494:THR:CG2	2.46	0.45
1:B:117:PRO:O	1:B:121:VAL:HG23	2.16	0.45
1:B:218:ASP:OD2	1:B:469:GLY:HA2	2.15	0.45
1:B:494:THR:HA	1:B:497:ILE:HG12	1.98	0.45
1:C:121:VAL:HA	1:C:124:GLN:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:VAL:HG22	1:C:268:GLN:N	2.31	0.45
1:C:360:ILE:HG23	1:C:364:PHE:CE2	2.50	0.45
1:C:638:LEU:HD11	1:C:713:SER:OG	2.16	0.45
1:A:208:VAL:CG2	1:A:577:ILE:HG21	2.45	0.45
1:A:244:LEU:HD23	1:A:455:VAL:HG12	1.97	0.45
1:A:305:ILE:HG13	1:A:306:LEU:N	2.30	0.45
1:A:538:ASN:ND2	1:B:535:LEU:O	2.50	0.45
1:A:642:VAL:HG22	1:A:706:ILE:CG2	2.47	0.45
1:B:86:MET:HE1	1:B:139:LEU:HD23	1.98	0.45
1:C:126:GLY:O	1:C:456:SER:HA	2.15	0.45
1:D:50:LEU:HD23	1:D:50:LEU:C	2.41	0.45
1:D:246:GLU:OE2	1:D:707:LYS:HE2	2.16	0.45
1:D:487:LEU:O	1:D:490:VAL:HG22	2.16	0.45
1:B:263:PHE:CB	1:B:283:ILE:HG13	2.46	0.45
1:B:494:THR:HA	1:B:497:ILE:CD1	2.46	0.45
1:C:318:GLN:CB	1:C:490:VAL:HG11	2.45	0.45
1:C:383:TYR:CE2	1:C:419:PRO:HG2	2.51	0.45
1:C:507:ILE:HD11	1:C:646:ALA:CB	2.46	0.45
1:D:123:TYR:OH	1:D:305:ILE:HA	2.16	0.45
1:A:416:SER:O	1:A:420:PRO:HD2	2.16	0.45
1:A:458:ASP:O	1:A:462:PRO:CD	2.63	0.45
1:A:491:GLY:C	1:A:494:THR:HG22	2.42	0.45
1:A:491:GLY:CA	1:A:494:THR:HG22	2.46	0.45
1:A:573:MET:CE	1:A:603:THR:CG2	2.94	0.45
1:A:682:LYS:O	1:A:686:ILE:HG13	2.17	0.45
1:B:138:LEU:CD1	1:B:295:LEU:HA	2.46	0.45
1:B:409:GLY:HA3	1:B:659:TRP:NE1	2.31	0.45
1:B:499:LYS:HE2	1:B:695:LYS:O	2.16	0.45
1:B:622:PRO:CG	1:B:709:MET:HG3	2.34	0.45
1:D:84:ALA:HB1	1:D:186:ILE:HG13	1.98	0.45
1:D:154:GLN:HE21	1:D:171:PRO:HB2	1.81	0.45
1:D:184:SER:OG	1:D:708:ILE:HG23	2.15	0.45
1:D:226:ILE:HG23	1:D:600:ILE:HD11	1.98	0.45
1:D:666:LEU:C	1:D:666:LEU:HD23	2.42	0.45
1:A:163:ASN:HB2	1:A:169:PHE:CE1	2.51	0.45
1:A:298:LEU:O	1:A:302:MET:HG3	2.16	0.45
1:B:218:ASP:HA	1:B:225:THR:CG2	2.47	0.45
1:B:224:ALA:HB2	1:B:577:ILE:HD11	1.98	0.45
1:B:252:ILE:HD13	1:B:445:LEU:CD2	2.46	0.45
1:C:129:MET:HE1	1:C:241:GLY:HA3	1.96	0.45
1:C:659:TRP:HB3	1:C:688:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ASP:OD1	1:D:206:ASP:OD2	2.35	0.45
1:D:376:ILE:HD11	1:D:424:LEU:HD21	1.98	0.45
1:A:254:SER:OG	1:A:512:SER:HB3	2.17	0.45
1:B:480:VAL:CG1	1:B:481:ARG:H	2.30	0.45
1:B:587:LEU:HA	1:B:592:ALA:HB3	1.98	0.45
1:C:393:PHE:CE1	1:D:571:MET:HE1	2.51	0.45
1:C:497:ILE:HG22	1:C:501:PHE:CE2	2.52	0.45
1:C:613:TYR:N	1:C:614:PRO:HD2	2.30	0.45
1:D:336:THR:HG22	1:D:363:TRP:CD1	2.49	0.45
1:D:424:LEU:HD13	1:D:508:PHE:HE1	1.82	0.45
1:D:445:LEU:HD12	1:D:445:LEU:O	2.17	0.45
1:A:355:PHE:CZ	1:A:362:PRO:HG3	2.51	0.45
1:A:536:LEU:HD12	1:B:538:ASN:HB2	1.98	0.45
1:A:702:LEU:O	1:A:706:ILE:HG13	2.17	0.45
1:B:312:LYS:CB	1:B:313:PRO:HD2	2.47	0.45
1:B:517:TYR:HE2	1:B:713:SER:HB3	1.82	0.45
1:B:625:THR:HB	1:B:633:PHE:CE2	2.51	0.45
1:C:511:LEU:HD11	1:D:545:ILE:HG21	1.98	0.45
1:D:73:THR:HG22	1:D:75:GLN:N	2.31	0.45
1:D:129:MET:C	1:D:129:MET:HE3	2.41	0.45
1:D:389:LYS:N	1:D:390:PRO:HD2	2.31	0.45
1:D:503:ILE:HG12	1:D:649:ALA:HB3	1.98	0.45
1:A:131:LEU:HD11	1:A:305:ILE:CD1	2.47	0.45
1:A:194:GLY:O	1:A:198:THR:HG22	2.17	0.45
1:A:199:LYS:HA	1:A:199:LYS:HD3	1.51	0.45
1:C:73:THR:O	1:C:76:THR:HB	2.17	0.45
1:C:192:VAL:CG1	1:C:611:MET:HA	2.47	0.45
1:D:208:VAL:HG21	1:D:577:ILE:CG2	2.46	0.45
1:D:265:ILE:HG22	1:D:522:ILE:HG21	1.99	0.45
1:D:488:ASP:HB3	2:D:801:ZOL:N17	2.32	0.45
1:D:547:GLY:O	1:D:637:VAL:HG22	2.16	0.45
1:A:82:LEU:HG	1:A:179:TYR:HE1	1.82	0.45
1:B:110:ARG:HG3	1:B:476:LEU:CG	2.46	0.45
1:B:130:GLY:HA2	1:B:455:VAL:CG1	2.47	0.45
1:D:129:MET:O	1:D:132:SER:OG	2.32	0.45
1:D:169:PHE:HB2	1:D:174:MET:CG	2.47	0.45
1:A:226:ILE:HG21	1:A:596:TYR:CB	2.46	0.45
1:B:678:SER:HB3	1:B:680:PRO:HD2	1.98	0.45
1:C:383:TYR:CZ	1:C:416:SER:HA	2.51	0.45
1:D:199:LYS:HD3	1:D:199:LYS:HA	1.76	0.45
1:D:299:GLY:O	1:D:303:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:CE	1:A:128:VAL:HG21	2.45	0.44
1:B:149:GLY:CA	1:B:155:VAL:HG23	2.46	0.44
1:B:188:MET:HB2	1:B:704:ILE:HG21	1.98	0.44
1:B:353:LEU:HD11	1:B:355:PHE:CD2	2.51	0.44
1:B:394:LEU:HD21	1:B:659:TRP:CD1	2.51	0.44
1:B:416:SER:CB	1:B:654:ASN:HD22	2.30	0.44
1:B:483:ILE:O	1:B:487:LEU:HG	2.17	0.44
1:C:80:PHE:HE2	1:C:181:LEU:HG	1.81	0.44
1:C:579:ARG:HA	1:C:582:ARG:HG2	1.99	0.44
1:C:597:ASN:CA	1:C:600:ILE:HG12	2.43	0.44
1:D:8:PHE:HD1	1:D:142:VAL:HG11	1.82	0.44
1:D:17:PHE:HD2	1:D:131:LEU:HD11	1.81	0.44
1:A:553:ALA:HB2	1:B:421:THR:CG2	2.44	0.44
1:C:564:SER:HB2	1:D:411:SER:OG	2.17	0.44
1:A:308:VAL:CG2	1:A:324:SER:HB2	2.47	0.44
1:A:321:LEU:HD13	1:A:457:VAL:HG13	1.98	0.44
1:B:138:LEU:HD21	1:B:294:ALA:CB	2.47	0.44
1:C:267:VAL:HG21	1:C:274:LEU:HB3	1.99	0.44
1:C:519:PHE:O	1:C:522:ILE:HG12	2.17	0.44
1:D:107:GLU:HA	1:D:110:ARG:HG2	2.00	0.44
1:A:22:PHE:HA	1:A:97:MET:HE1	2.00	0.44
1:A:216:PRO:O	1:A:219:ASP:HB2	2.16	0.44
1:A:219:ASP:OD1	1:A:220:PRO:HD2	2.17	0.44
1:A:223:PRO:HG2	1:A:577:ILE:HD13	1.97	0.44
1:A:253:VAL:CG1	1:A:257:ILE:CD1	2.96	0.44
1:A:302:MET:HA	1:A:305:ILE:HG12	1.98	0.44
1:B:86:MET:HE2	1:B:136:PHE:O	2.17	0.44
1:C:517:TYR:CB	1:C:714:VAL:HG22	2.35	0.44
1:C:539:MET:HE2	1:D:639:ILE:CG2	2.48	0.44
1:D:31:GLY:HA3	1:D:107:GLU:HB2	1.99	0.44
1:A:138:LEU:HD12	1:A:298:LEU:CD1	2.41	0.44
1:A:337:ALA:HB2	1:A:363:TRP:CE2	2.53	0.44
1:A:409:GLY:HA3	1:A:659:TRP:CE2	2.53	0.44
1:A:477:ASP:O	1:A:480:VAL:HG22	2.17	0.44
1:B:627:PHE:CE1	1:B:720:PHE:HB3	2.52	0.44
1:C:363:TRP:CE2	1:C:367:ILE:HD11	2.53	0.44
1:C:519:PHE:CE1	1:C:535:LEU:HD21	2.52	0.44
1:D:134:GLY:O	1:D:138:LEU:HD23	2.17	0.44
1:D:550:LEU:HG	1:D:633:PHE:HZ	1.82	0.44
1:D:703:ASP:O	1:D:707:LYS:HG3	2.18	0.44
1:A:691:GLY:O	1:A:695:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ILE:O	1:B:712:VAL:HG23	2.18	0.44
1:C:57:ILE:CD1	1:C:189:PHE:HB3	2.48	0.44
1:C:692:ASP:O	1:C:695:LYS:HG2	2.16	0.44
1:A:47:ASP:OD1	1:A:95:MET:HE1	2.18	0.44
1:A:194:GLY:HA3	1:A:235:GLY:CA	2.41	0.44
1:A:263:PHE:CB	1:A:283:ILE:HG13	2.46	0.44
1:B:18:ALA:HB2	1:B:131:LEU:HB2	2.00	0.44
1:C:218:ASP:HA	1:C:225:THR:HG22	1.99	0.44
1:D:457:VAL:HG11	1:D:494:THR:HG21	1.99	0.44
1:A:176:VAL:CG2	1:A:253:VAL:HG22	2.47	0.44
1:A:719:ILE:O	1:A:723:VAL:HG23	2.18	0.44
1:B:74:TRP:CE2	1:B:75:GLN:HG3	2.53	0.44
1:B:88:ALA:O	1:B:92:ILE:CD1	2.66	0.44
1:C:366:ALA:HB2	1:C:442:ILE:HG22	1.99	0.44
1:C:507:ILE:HD11	1:C:646:ALA:HB1	2.00	0.44
1:D:69:MET:HA	1:D:74:TRP:HA	1.99	0.44
1:D:216:PRO:HG2	1:D:219:ASP:HB2	1.99	0.44
1:A:10:ILE:N	1:A:11:PRO:HD2	2.32	0.44
1:A:21:ASN:ND2	1:A:127:SER:OG	2.50	0.44
1:B:126:GLY:C	1:B:456:SER:HA	2.43	0.44
1:C:42:ILE:HG23	1:C:230:VAL:CG1	2.47	0.44
1:C:231:GLY:HA2	1:C:234:VAL:CG1	2.47	0.44
1:D:176:VAL:HB	1:D:253:VAL:CG1	2.42	0.44
1:A:40:SER:O	1:A:43:ARG:HG2	2.18	0.43
1:A:202:ASP:OD1	1:A:692:ASP:OD2	2.36	0.43
1:B:252:ILE:O	1:B:256:ILE:HG12	2.17	0.43
1:B:480:VAL:CG1	1:B:481:ARG:N	2.80	0.43
1:C:50:LEU:HD21	1:C:92:ILE:HG12	2.00	0.43
1:C:597:ASN:O	1:C:600:ILE:HG12	2.18	0.43
1:D:402:THR:HA	1:D:683:ALA:HB1	2.00	0.43
1:B:8:PHE:O	1:B:11:PRO:HD2	2.18	0.43
1:B:197:TYR:OH	1:B:600:ILE:HG23	2.18	0.43
1:C:119:LEU:HD23	1:C:317:PRO:HB2	1.99	0.43
1:C:258:LEU:HD23	1:C:438:TYR:HA	2.00	0.43
1:C:717:VAL:HA	1:C:720:PHE:CZ	2.54	0.43
1:D:14:ALA:HB2	1:D:302:MET:SD	2.59	0.43
1:D:18:ALA:HB2	1:D:131:LEU:HB2	1.99	0.43
1:D:619:ILE:O	1:D:622:PRO:HD2	2.18	0.43
1:B:514:PHE:HE1	1:B:638:LEU:HB3	1.83	0.43
1:C:630:GLY:O	1:C:634:VAL:HG23	2.18	0.43
1:D:107:GLU:HG2	1:D:108:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LEU:CD1	1:D:295:LEU:HD23	2.47	0.43
1:D:711:VAL:O	1:D:714:VAL:HG12	2.18	0.43
1:A:571:MET:HG2	1:B:400:GLU:HG3	2.01	0.43
1:A:686:ILE:HD13	1:B:402:THR:HB	2.00	0.43
1:B:198:THR:HG23	1:B:199:LYS:N	2.32	0.43
1:B:265:ILE:CD1	1:B:522:ILE:HG21	2.48	0.43
1:C:230:VAL:O	1:C:234:VAL:HG12	2.19	0.43
1:C:539:MET:HE2	1:D:639:ILE:HG21	2.00	0.43
1:D:244:LEU:HD22	1:D:455:VAL:HG22	1.97	0.43
1:D:293:PHE:CE2	1:D:445:LEU:HG	2.53	0.43
1:A:296:VAL:HG13	1:A:335:LEU:HD22	2.01	0.43
1:A:565:ALA:HB2	1:A:610:GLN:OE1	2.19	0.43
1:B:244:LEU:HG	1:B:451:VAL:CG2	2.48	0.43
1:C:500:GLY:O	1:C:503:ILE:HG22	2.17	0.43
1:C:707:LYS:O	1:C:711:VAL:HG23	2.19	0.43
1:D:561:TYR:HE2	1:D:614:PRO:HD3	1.84	0.43
1:A:118:ALA:O	1:A:121:VAL:HG12	2.18	0.43
1:A:131:LEU:HD21	1:A:305:ILE:HD13	2.00	0.43
1:A:131:LEU:HD11	1:A:305:ILE:HD11	2.01	0.43
1:A:268:GLN:HB2	1:A:277:GLN:OE1	2.19	0.43
1:A:416:SER:CB	1:A:654:ASN:HD22	2.32	0.43
1:A:480:VAL:O	1:A:484:THR:HG23	2.19	0.43
1:A:522:ILE:HD11	1:A:534:VAL:HG11	1.99	0.43
1:B:84:ALA:CB	1:B:186:ILE:HG13	2.45	0.43
1:C:365:SER:O	1:C:443:ALA:HB2	2.19	0.43
1:C:647:MET:HE2	1:C:647:MET:N	2.34	0.43
1:D:693:PRO:O	1:D:697:THR:HB	2.19	0.43
1:A:306:LEU:O	1:A:309:ILE:HG12	2.19	0.43
1:B:25:VAL:HG21	1:B:124:GLN:CG	2.49	0.43
1:B:50:LEU:HD22	1:B:95:MET:HE2	2.01	0.43
1:B:298:LEU:HD23	1:B:298:LEU:C	2.43	0.43
1:C:165:LEU:HG	1:C:165:LEU:O	2.19	0.43
1:C:226:ILE:HD12	1:C:596:TYR:CG	2.54	0.43
1:D:69:MET:HG3	1:D:77:GLY:HA3	2.01	0.43
1:A:115:ILE:HD12	1:A:115:ILE:H	1.82	0.43
1:A:493:THR:O	1:A:497:ILE:HG13	2.19	0.43
1:B:482:LYS:HD3	1:B:483:ILE:N	2.34	0.43
1:D:258:LEU:HD11	1:D:437:LEU:HB2	2.01	0.43
1:A:359:ALA:O	1:A:362:PRO:HD2	2.19	0.43
1:B:138:LEU:HD13	1:B:295:LEU:HA	2.01	0.43
1:C:53:GLU:OE2	1:C:193:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ALA:O	1:C:230:VAL:HG22	2.18	0.43
1:C:539:MET:CE	1:C:545:ILE:HA	2.49	0.43
1:D:86:MET:HE2	1:D:136:PHE:O	2.19	0.43
1:D:412:LEU:HD23	1:D:412:LEU:C	2.44	0.43
1:A:122:ALA:HB3	1:A:460:TYR:CE1	2.54	0.43
1:A:317:PRO:O	1:A:321:LEU:HG	2.19	0.43
1:A:537:LEU:HD23	1:A:639:ILE:HD11	2.01	0.43
1:B:65:ALA:HB2	1:B:81:LEU:CD2	2.48	0.43
1:B:145:TYR:HA	1:B:172:PHE:CZ	2.54	0.43
1:B:402:THR:HA	1:B:683:ALA:HB1	2.00	0.43
1:C:504:GLY:O	1:C:508:PHE:HD2	2.02	0.43
1:A:164:TRP:CE3	1:A:165:LEU:HB2	2.53	0.42
1:A:300:CYS:HB3	1:A:332:THR:OG1	2.19	0.42
1:B:261:TYR:O	1:B:265:ILE:HG12	2.19	0.42
1:D:289:TYR:N	1:D:290:PRO:HD2	2.34	0.42
1:B:41:TYR:OH	1:B:597:ASN:OD1	2.32	0.42
1:B:115:ILE:CG2	1:B:487:LEU:HD21	2.48	0.42
1:B:439:GLY:HA2	1:B:442:ILE:HG22	2.01	0.42
1:C:252:ILE:HG12	1:C:445:LEU:HD13	1.99	0.42
1:D:6:LEU:O	1:D:10:ILE:HG13	2.18	0.42
1:A:148:PHE:O	1:A:152:MET:HB2	2.18	0.42
1:A:266:TYR:O	1:A:277:GLN:HB2	2.19	0.42
1:A:327:THR:O	1:A:331:LEU:HG	2.19	0.42
1:A:416:SER:O	1:A:419:PRO:HD2	2.20	0.42
1:A:538:ASN:HB2	1:B:536:LEU:CD1	2.43	0.42
1:B:204:ALA:HA	1:B:574:VAL:CG2	2.48	0.42
1:C:9:LEU:HD12	1:C:12:LEU:HD12	2.00	0.42
1:C:469:GLY:O	1:C:473:MET:HG2	2.20	0.42
1:D:102:ASN:O	1:D:105:VAL:HG12	2.20	0.42
1:D:199:LYS:HE3	1:D:696:ASP:HB2	2.01	0.42
1:A:65:ALA:HB2	1:A:81:LEU:CD2	2.49	0.42
1:A:105:VAL:HG23	1:A:121:VAL:CG1	2.49	0.42
1:B:15:LEU:CD2	1:B:135:GLY:HA3	2.49	0.42
1:B:23:ALA:C	1:B:26:VAL:HG12	2.44	0.42
1:B:145:TYR:HA	1:B:172:PHE:HZ	1.83	0.42
1:B:189:PHE:CZ	1:B:615:ALA:HB3	2.54	0.42
1:B:705:LEU:O	1:B:708:ILE:HG22	2.19	0.42
1:C:58:PHE:HE1	1:C:85:VAL:HG22	1.83	0.42
1:C:419:PRO:CB	1:C:420:PRO:HD3	2.47	0.42
1:C:698:VAL:O	1:C:702:LEU:HG	2.19	0.42
1:D:459:SER:O	1:D:462:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:682:LYS:O	1:D:686:ILE:HG13	2.19	0.42
1:A:191:ARG:HH21	1:A:240:LEU:N	2.16	0.42
1:B:494:THR:C	1:B:497:ILE:HG12	2.44	0.42
1:C:231:GLY:HA2	1:C:234:VAL:HG12	2.02	0.42
1:C:245:LEU:C	1:C:245:LEU:HD23	2.45	0.42
1:C:633:PHE:O	1:C:637:VAL:HG23	2.20	0.42
1:D:131:LEU:HD22	1:D:302:MET:HG2	2.01	0.42
1:D:460:TYR:HA	1:D:463:ILE:CD1	2.49	0.42
1:A:86:MET:HE3	1:A:136:PHE:HB3	2.02	0.42
1:A:700:PRO:O	1:A:703:ASP:OD1	2.38	0.42
1:B:398:SER:HB3	1:B:684:LEU:HD13	2.02	0.42
1:C:377:GLY:O	1:C:497:ILE:HG12	2.20	0.42
1:D:79:ALA:HB1	1:D:179:TYR:HB2	2.00	0.42
1:A:66:ILE:O	1:A:70:ILE:HG13	2.19	0.42
1:A:120:LYS:HD3	1:A:313:PRO:HB3	2.02	0.42
1:A:198:THR:HG23	1:A:199:LYS:N	2.34	0.42
1:A:680:PRO:O	1:A:684:LEU:HD23	2.19	0.42
1:B:618:ALA:HB1	1:B:708:ILE:HG21	2.01	0.42
1:C:320:GLU:HA	1:C:323:ILE:HD12	2.01	0.42
1:C:587:LEU:HD11	1:C:594:PRO:HB3	2.01	0.42
1:D:107:GLU:HA	1:D:110:ARG:CG	2.49	0.42
1:D:169:PHE:CD2	1:D:174:MET:HG3	2.54	0.42
1:D:641:THR:HG22	1:D:706:ILE:HG12	2.00	0.42
1:A:181:LEU:O	1:A:185:ILE:HG12	2.20	0.42
1:A:184:SER:OG	1:A:708:ILE:HB	2.19	0.42
1:C:305:ILE:O	1:C:309:ILE:HG23	2.20	0.42
1:C:426:LEU:C	1:C:426:LEU:HD23	2.45	0.42
1:D:451:VAL:HG22	1:D:455:VAL:HG23	2.02	0.42
1:A:151:TRP:CZ3	1:A:152:MET:HE2	2.55	0.42
1:A:471:SER:HA	1:A:476:LEU:CD1	2.48	0.42
1:B:223:PRO:HB3	1:B:594:PRO:HB2	2.02	0.42
1:C:169:PHE:HB2	1:C:174:MET:CG	2.49	0.42
1:D:41:TYR:CE2	1:D:226:ILE:HG12	2.55	0.42
1:D:129:MET:HE3	1:D:129:MET:O	2.19	0.42
1:D:227:ALA:HA	1:D:230:VAL:CG1	2.50	0.42
1:D:240:LEU:HD21	1:D:458:ASP:CB	2.43	0.42
1:D:293:PHE:HD2	1:D:445:LEU:CD2	2.33	0.42
1:D:298:LEU:C	1:D:298:LEU:HD23	2.45	0.42
1:D:379:TRP:CD2	1:D:419:PRO:HB3	2.54	0.42
1:D:504:GLY:O	1:D:508:PHE:HD1	2.02	0.42
1:D:663:LYS:CA	1:D:684:LEU:HD21	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:PHE:CD2	1:A:131:LEU:HD11	2.55	0.42
1:A:57:ILE:CG2	1:A:186:ILE:HD13	2.50	0.42
1:A:164:TRP:O	1:A:165:LEU:HB3	2.20	0.42
1:B:95:MET:HA	1:B:237:VAL:HG11	2.00	0.42
1:C:122:ALA:HB1	1:C:460:TYR:HB2	2.01	0.42
1:C:292:PHE:HA	1:C:295:LEU:HD12	2.02	0.42
1:C:659:TRP:HE3	1:C:691:GLY:HA3	1.84	0.42
1:D:660:ASP:O	1:D:664:LYS:HG3	2.19	0.42
1:D:679:GLU:HB2	1:D:680:PRO:HD3	2.02	0.42
1:D:708:ILE:HG13	1:D:709:MET:N	2.34	0.42
1:A:213:LEU:CB	1:A:215:LEU:HD13	2.49	0.41
1:A:380:ALA:O	1:A:384:THR:HG22	2.19	0.41
1:A:666:LEU:HD23	1:A:666:LEU:C	2.45	0.41
1:B:317:PRO:CD	1:B:486:HIS:HE1	2.33	0.41
1:B:482:LYS:HD3	1:B:482:LYS:C	2.44	0.41
1:B:566:VAL:HG11	1:B:693:PRO:HB3	2.01	0.41
1:B:620:LEU:O	1:B:624:VAL:HG22	2.20	0.41
1:B:659:TRP:HB3	5:B:905:HOH:O	2.19	0.41
1:D:383:TYR:HE2	1:D:419:PRO:HG2	1.85	0.41
1:A:21:ASN:OD1	1:A:124:GLN:NE2	2.53	0.41
1:B:57:ILE:HD12	1:B:186:ILE:HG23	2.01	0.41
1:C:164:TRP:O	1:C:165:LEU:HB3	2.20	0.41
1:D:563:ILE:O	1:D:567:THR:HG23	2.20	0.41
1:D:666:LEU:HD23	1:D:666:LEU:O	2.20	0.41
1:D:709:MET:HE3	1:D:709:MET:HB2	1.86	0.41
1:B:174:MET:HE2	1:B:174:MET:HA	2.01	0.41
1:B:289:TYR:N	1:B:290:PRO:HD2	2.36	0.41
1:B:306:LEU:C	1:B:306:LEU:HD23	2.45	0.41
1:C:232:ASP:O	1:C:237:VAL:HG23	2.20	0.41
1:C:425:VAL:HG11	1:D:550:LEU:CD2	2.49	0.41
1:D:105:VAL:HG13	1:D:467:ALA:HB2	2.02	0.41
1:D:413:GLY:HA3	1:D:655:SER:HB3	2.02	0.41
1:B:124:GLN:NE2	1:B:309:ILE:HD11	2.35	0.41
1:B:476:LEU:HD23	1:B:480:VAL:HG11	2.02	0.41
1:B:671:LEU:CD2	1:B:674:TYR:HD2	2.33	0.41
1:C:540:LEU:HD21	1:D:518:MET:CG	2.41	0.41
1:D:31:GLY:CA	1:D:107:GLU:HB2	2.50	0.41
1:A:163:ASN:HB3	1:A:167:ILE:HB	2.02	0.41
1:A:185:ILE:HD13	1:A:708:ILE:HD11	2.02	0.41
1:A:567:THR:HG22	1:B:407:SER:CB	2.50	0.41
1:B:319:ARG:O	1:B:323:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:GLY:HA3	1:C:497:ILE:CG2	2.32	0.41
1:C:600:ILE:HG13	1:C:601:GLU:N	2.34	0.41
1:D:424:LEU:O	1:D:428:ILE:HG13	2.20	0.41
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.88	0.41
1:A:296:VAL:CG2	1:A:339:LEU:HD22	2.50	0.41
1:A:567:THR:HG22	1:B:407:SER:HB3	2.03	0.41
1:B:587:LEU:CD1	1:B:594:PRO:HD3	2.50	0.41
1:B:618:ALA:HB1	1:B:708:ILE:CG2	2.50	0.41
1:D:198:THR:HG23	1:D:199:LYS:N	2.36	0.41
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.90	0.41
1:A:298:LEU:HD23	1:A:298:LEU:C	2.46	0.41
1:B:254:SER:OG	1:B:512:SER:HB3	2.20	0.41
1:B:288:SER:HB2	1:B:292:PHE:CE2	2.55	0.41
1:B:444:ALA:HB2	1:B:508:PHE:HB2	1.99	0.41
1:C:188:MET:SD	1:C:615:ALA:HA	2.60	0.41
1:D:149:GLY:HA2	1:D:154:GLN:HB2	2.02	0.41
1:A:257:ILE:HA	1:A:260:SER:OG	2.20	0.41
1:B:148:PHE:O	1:B:152:MET:HB2	2.21	0.41
1:B:293:PHE:CE1	1:B:336:THR:HG21	2.56	0.41
1:B:521:GLN:HG2	1:B:717:VAL:HG21	2.02	0.41
1:C:355:PHE:CE1	1:C:362:PRO:HD3	2.56	0.41
1:C:424:LEU:O	1:C:428:ILE:HG13	2.20	0.41
1:C:457:VAL:O	1:C:460:TYR:CD1	2.74	0.41
1:D:21:ASN:HB2	1:D:128:VAL:CG1	2.48	0.41
1:D:141:LEU:CD2	1:D:252:ILE:HG21	2.51	0.41
1:D:355:PHE:HE1	1:D:362:PRO:HD3	1.85	0.41
1:D:466:ASN:O	1:D:470:ILE:HG13	2.21	0.41
1:D:492:ASN:OD1	1:D:493:THR:N	2.53	0.41
1:A:73:THR:OG1	1:A:75:GLN:HG2	2.20	0.41
1:A:204:ALA:CB	1:A:573:MET:HB3	2.50	0.41
1:A:300:CYS:HB3	1:A:332:THR:HG1	1.86	0.41
1:A:678:SER:HB2	1:A:680:PRO:HD2	2.03	0.41
1:B:15:LEU:HD22	1:B:135:GLY:HA3	2.03	0.41
1:B:130:GLY:HA2	1:B:455:VAL:CB	2.50	0.41
1:C:79:ALA:HB1	1:C:179:TYR:HB2	2.03	0.41
1:C:263:PHE:HB3	1:C:264:PRO:HD3	2.02	0.41
1:C:573:MET:O	1:C:577:ILE:HG13	2.20	0.41
1:C:596:TYR:O	1:C:600:ILE:HG23	2.20	0.41
1:C:665:TYR:CD1	1:C:670:ASN:HB2	2.56	0.41
1:D:32:THR:HG23	1:D:35:MET:H	1.85	0.41
1:D:208:VAL:HA	1:D:212:GLU:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ALA:HA	1:D:470:ILE:HD12	2.03	0.41
1:D:563:ILE:HD13	1:D:693:PRO:HB2	2.03	0.41
1:A:249:VAL:O	1:A:253:VAL:HG23	2.21	0.41
1:A:325:LEU:HD12	1:A:326:TRP:CD1	2.56	0.41
1:A:717:VAL:HA	1:A:720:PHE:CZ	2.56	0.41
1:B:78:VAL:HG11	1:B:148:PHE:CZ	2.56	0.41
1:B:350:LEU:HB3	1:B:355:PHE:HD2	1.86	0.41
1:B:370:ILE:HG12	1:B:446:GLY:O	2.21	0.41
1:B:460:TYR:OH	1:B:487:LEU:HD22	2.20	0.41
1:A:75:GLN:HB2	1:A:148:PHE:CD1	2.56	0.40
1:A:222:ASN:OD1	1:A:223:PRO:HD2	2.21	0.40
1:B:169:PHE:CD2	1:B:174:MET:HG3	2.56	0.40
1:C:163:ASN:N	1:C:167:ILE:O	2.54	0.40
1:C:192:VAL:HG12	1:C:611:MET:HA	2.02	0.40
1:C:229:ASN:ND2	1:C:473:MET:HE3	2.35	0.40
1:C:451:VAL:O	1:C:455:VAL:HG23	2.22	0.40
1:D:288:SER:HB2	1:D:292:PHE:HE2	1.86	0.40
1:D:622:PRO:CG	1:D:709:MET:HG3	2.49	0.40
1:A:624:VAL:HG23	1:A:625:THR:N	2.37	0.40
1:B:130:GLY:CA	1:B:455:VAL:HB	2.50	0.40
1:C:129:MET:HE2	1:C:241:GLY:HA3	2.02	0.40
1:C:651:LEU:C	1:C:651:LEU:HD23	2.46	0.40
1:A:176:VAL:HG22	1:A:253:VAL:CG1	2.48	0.40
1:A:197:TYR:CE1	1:A:230:VAL:HG23	2.56	0.40
1:A:452:ALA:O	1:A:455:VAL:CG2	2.69	0.40
1:A:705:LEU:HA	1:A:708:ILE:HG22	2.02	0.40
1:B:10:ILE:HG22	1:B:298:LEU:HD22	2.02	0.40
1:B:624:VAL:HG23	1:B:625:THR:N	2.36	0.40
1:C:200:ALA:HB1	1:C:569:ALA:HB3	2.03	0.40
1:C:262:MET:CE	1:C:353:LEU:HD13	2.52	0.40
1:C:548:ALA:HB1	1:D:643:LEU:HD11	2.02	0.40
1:D:3:VAL:O	1:D:3:VAL:HG12	2.20	0.40
1:D:17:PHE:HB3	1:D:131:LEU:HD13	2.03	0.40
1:D:191:ARG:HH21	1:D:240:LEU:N	2.18	0.40
1:D:248:PHE:CZ	1:D:294:ALA:HB1	2.56	0.40
1:A:97:MET:CE	1:A:128:VAL:HG11	2.51	0.40
1:B:704:ILE:O	1:B:708:ILE:HG22	2.22	0.40
1:C:511:LEU:CD1	1:D:545:ILE:HD13	2.41	0.40
1:D:245:LEU:HD23	1:D:245:LEU:C	2.45	0.40
1:A:561:TYR:HA	1:B:415:LYS:HE3	2.04	0.40
1:B:79:ALA:HB1	1:B:179:TYR:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:PRO:HG3	1:C:473:MET:CA	2.38	0.40
1:C:308:VAL:CG2	1:C:324:SER:HB3	2.51	0.40
1:C:327:THR:HA	1:C:330:LEU:HG	2.04	0.40
1:D:127:SER:CB	1:D:305:ILE:HG21	2.50	0.40
1:D:188:MET:HG2	1:D:615:ALA:CB	2.51	0.40
1:D:188:MET:CG	1:D:615:ALA:HB2	2.52	0.40
1:D:599:CYS:O	1:D:603:THR:HG23	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	720/735 (98%)	710 (99%)	10 (1%)	0	100	100
1	B	710/735 (97%)	697 (98%)	13 (2%)	0	100	100
1	C	710/735 (97%)	702 (99%)	8 (1%)	0	100	100
1	D	706/735 (96%)	695 (98%)	11 (2%)	0	100	100
All	All	2846/2940 (97%)	2804 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	523/575 (91%)	518 (99%)	5 (1%)	68	75
1	B	513/575 (89%)	509 (99%)	4 (1%)	73	78
1	C	518/575 (90%)	515 (99%)	3 (1%)	78	81
1	D	507/575 (88%)	504 (99%)	3 (1%)	78	81
All	All	2061/2300 (90%)	2046 (99%)	15 (1%)	76	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	LEU
1	A	367	ILE
1	A	480	VAL
1	A	484	THR
1	A	719	ILE
1	B	258	LEU
1	B	267	VAL
1	B	719	ILE
1	B	725	LEU
1	C	471	SER
1	C	476	LEU
1	C	719	ILE
1	D	352	VAL
1	D	353	LEU
1	D	719	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	ASN
1	A	273	ASN
1	A	284	GLN
1	A	597	ASN
1	A	654	ASN
1	B	466	ASN
1	B	486	HIS
1	B	722	HIS
1	C	214	ASN
1	C	222	ASN
1	C	229	ASN
1	C	233	ASN

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Mol	Chain	Res	Type
1	C	606	ASN
1	C	722	HIS
1	D	21	ASN
1	D	233	ASN
1	D	276	HIS
1	D	318	GLN
1	D	681	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 16 are monoatomic - leaving 5 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
2	ZOL	B	801	3	16,16,16	5.89	4 (25%)	23,26,26	2.07	4 (17%)
4	LMT	D	806	-	36,36,36	1.04	3 (8%)	47,47,47	0.93	1 (2%)
2	ZOL	C	801	3	16,16,16	6.38	4 (25%)	23,26,26	1.93	4 (17%)
2	ZOL	D	801	3	16,16,16	5.95	4 (25%)	23,26,26	1.92	3 (13%)
2	ZOL	A	801	3	16,16,16	6.37	3 (18%)	23,26,26	2.15	5 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZOL	B	801	3	-	14/23/23/23	0/1/1/1
4	LMT	D	806	-	-	12/21/61/61	0/2/2/2
2	ZOL	C	801	3	-	3/23/23/23	0/1/1/1
2	ZOL	D	801	3	-	11/23/23/23	0/1/1/1
2	ZOL	A	801	3	-	19/23/23/23	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ZOL	P9-C8	19.08	1.98	1.85
2	A	801	ZOL	P14-C8	17.78	1.97	1.85
2	B	801	ZOL	P14-C8	17.65	1.97	1.85
2	A	801	ZOL	P9-C8	17.45	1.97	1.85
2	D	801	ZOL	P14-C8	16.67	1.96	1.85
2	D	801	ZOL	P9-C8	16.21	1.96	1.85
2	C	801	ZOL	P14-C8	16.04	1.96	1.85
2	B	801	ZOL	P9-C8	14.78	1.95	1.85
2	A	801	ZOL	C19-C18	2.51	1.41	1.35
2	D	801	ZOL	C7-C8	2.43	1.57	1.54
2	B	801	ZOL	C19-C18	2.36	1.40	1.35
2	C	801	ZOL	C19-C18	2.30	1.40	1.35
2	D	801	ZOL	C19-C18	2.21	1.40	1.35
4	D	806	LMT	O5B-C5B	2.12	1.49	1.44
2	C	801	ZOL	C7-C8	2.11	1.57	1.54
4	D	806	LMT	O5B-C1B	2.10	1.47	1.41
2	B	801	ZOL	O13-C8	-2.04	1.42	1.44
4	D	806	LMT	O5'-C5'	2.01	1.49	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ZOL	P9-C8-P14	7.96	126.97	112.72
2	D	801	ZOL	P9-C8-P14	6.79	124.88	112.72
2	A	801	ZOL	P9-C8-P14	6.67	124.67	112.72
2	C	801	ZOL	P9-C8-P14	5.79	123.10	112.72
2	C	801	ZOL	C8-C7-N15	5.15	120.21	113.67
2	A	801	ZOL	C8-C7-N15	5.10	120.15	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ZOL	C8-C7-N15	3.76	118.44	113.67
2	A	801	ZOL	P9-C8-O13	-3.23	100.02	107.42
2	B	801	ZOL	P9-C8-O13	-2.41	101.89	107.42
2	A	801	ZOL	O11-P9-O10	2.32	114.78	108.24
2	D	801	ZOL	O11-P9-O10	2.30	114.72	108.24
2	B	801	ZOL	O11-P9-O10	2.29	114.71	108.24
2	C	801	ZOL	O11-P9-O10	2.27	114.63	108.24
2	B	801	ZOL	O12-P9-C8	-2.26	104.03	109.82
4	D	806	LMT	C1B-O1B-C4'	-2.25	112.66	117.98
2	C	801	ZOL	O12-P9-C8	-2.13	104.36	109.82
2	A	801	ZOL	O12-P9-C8	-2.00	104.68	109.82

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ZOL	P9-C8-P14-O17
2	A	801	ZOL	O13-C8-P14-O17
2	A	801	ZOL	P9-C8-P14-O16
2	A	801	ZOL	P9-C8-P14-O15
2	A	801	ZOL	P14-C8-P9-O10
2	A	801	ZOL	P14-C8-P9-O12
2	A	801	ZOL	O13-C8-P9-O10
2	A	801	ZOL	O13-C8-P9-O11
2	A	801	ZOL	O13-C8-P9-O12
2	A	801	ZOL	C7-C8-P9-O10
2	A	801	ZOL	C7-C8-P9-O11
2	A	801	ZOL	C7-C8-P9-O12
2	A	801	ZOL	N15-C7-C8-P9
2	B	801	ZOL	P9-C8-P14-O17
2	B	801	ZOL	O13-C8-P14-O17
2	B	801	ZOL	C7-C8-P14-O17
2	B	801	ZOL	P9-C8-P14-O16
2	B	801	ZOL	O13-C8-P14-O16
2	B	801	ZOL	C7-C8-P14-O16
2	B	801	ZOL	P9-C8-P14-O15
2	B	801	ZOL	O13-C8-P14-O15
2	B	801	ZOL	C7-C8-P14-O15
2	B	801	ZOL	O13-C8-P9-O12
2	B	801	ZOL	N15-C7-C8-P9
2	D	801	ZOL	O13-C8-P9-O12
2	D	801	ZOL	N15-C7-C8-P14

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Mol	Chain	Res	Type	Atoms
4	D	806	LMT	O5'-C1'-O1'-C1
4	D	806	LMT	C2-C3-C4-C5
4	D	806	LMT	C1-C2-C3-C4
2	A	801	ZOL	O13-C8-P14-O16
2	A	801	ZOL	P14-C8-P9-O11
2	D	801	ZOL	P14-C8-P9-O11
2	D	801	ZOL	O13-C8-P9-O10
4	D	806	LMT	C2B-C1B-O1B-C4'
4	D	806	LMT	C2-C1-O1'-C1'
4	D	806	LMT	C9-C10-C11-C12
4	D	806	LMT	O5B-C1B-O1B-C4'
4	D	806	LMT	C4-C5-C6-C7
4	D	806	LMT	C5'-C4'-O1B-C1B
2	A	801	ZOL	O13-C8-P14-O15
2	A	801	ZOL	N15-C7-C8-P14
2	B	801	ZOL	N15-C7-C8-P14
2	D	801	ZOL	P14-C8-P9-O12
2	D	801	ZOL	O13-C8-P9-O11
2	A	801	ZOL	C7-C8-P14-O17
2	A	801	ZOL	C7-C8-P14-O16
4	D	806	LMT	C3'-C4'-O1B-C1B
2	C	801	ZOL	P9-C8-P14-O16
2	C	801	ZOL	O13-C8-P14-O16
2	D	801	ZOL	P14-C8-P9-O10
2	D	801	ZOL	C7-C8-P9-O11
4	D	806	LMT	O5'-C5'-C6'-O6'
2	B	801	ZOL	P14-C8-P9-O10
2	B	801	ZOL	O13-C8-P9-O10
2	C	801	ZOL	P9-C8-P14-O15
2	D	801	ZOL	O13-C8-P14-O15
2	D	801	ZOL	C7-C8-P9-O12
2	D	801	ZOL	C8-C7-N15-C16
4	D	806	LMT	C11-C10-C9-C8

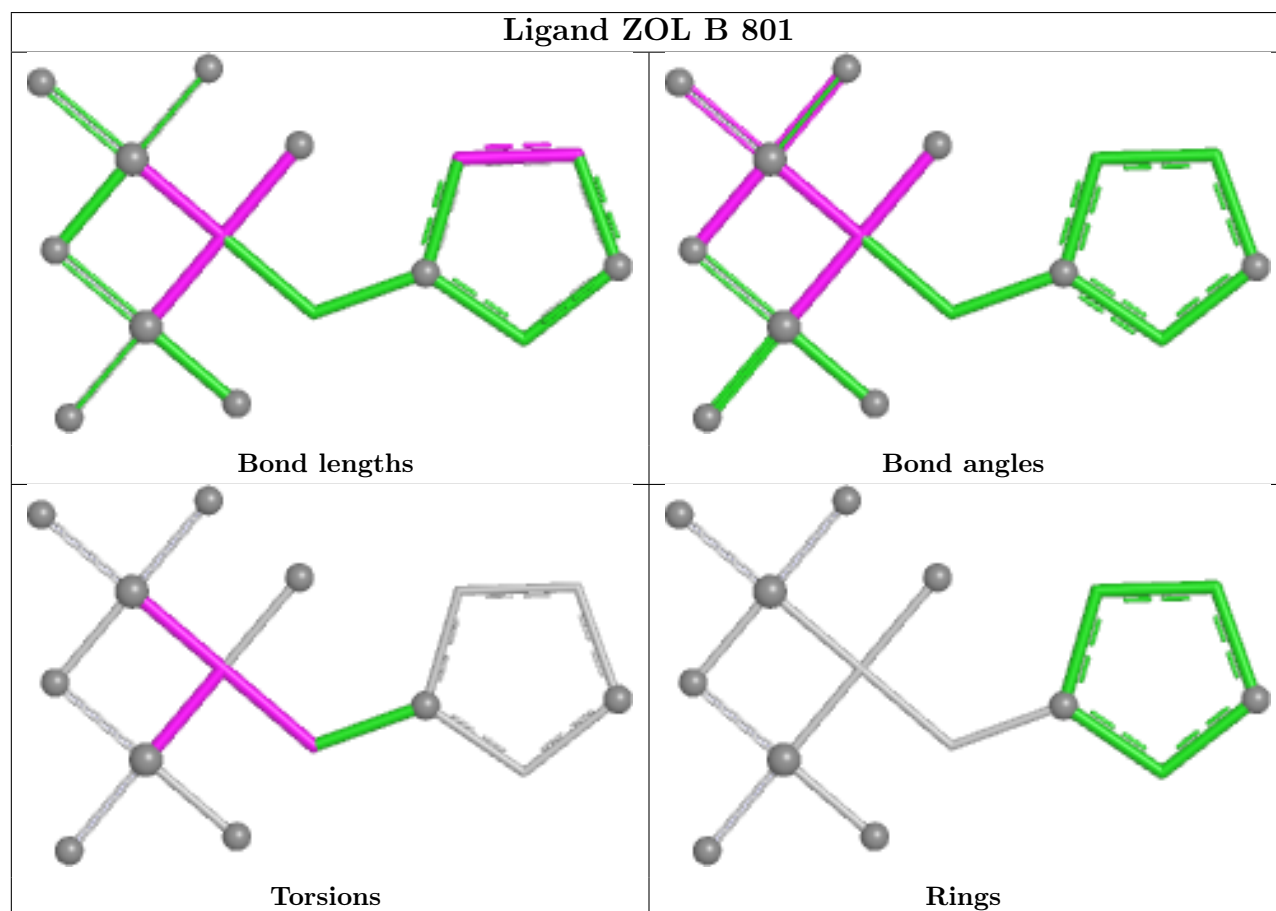
There are no ring outliers.

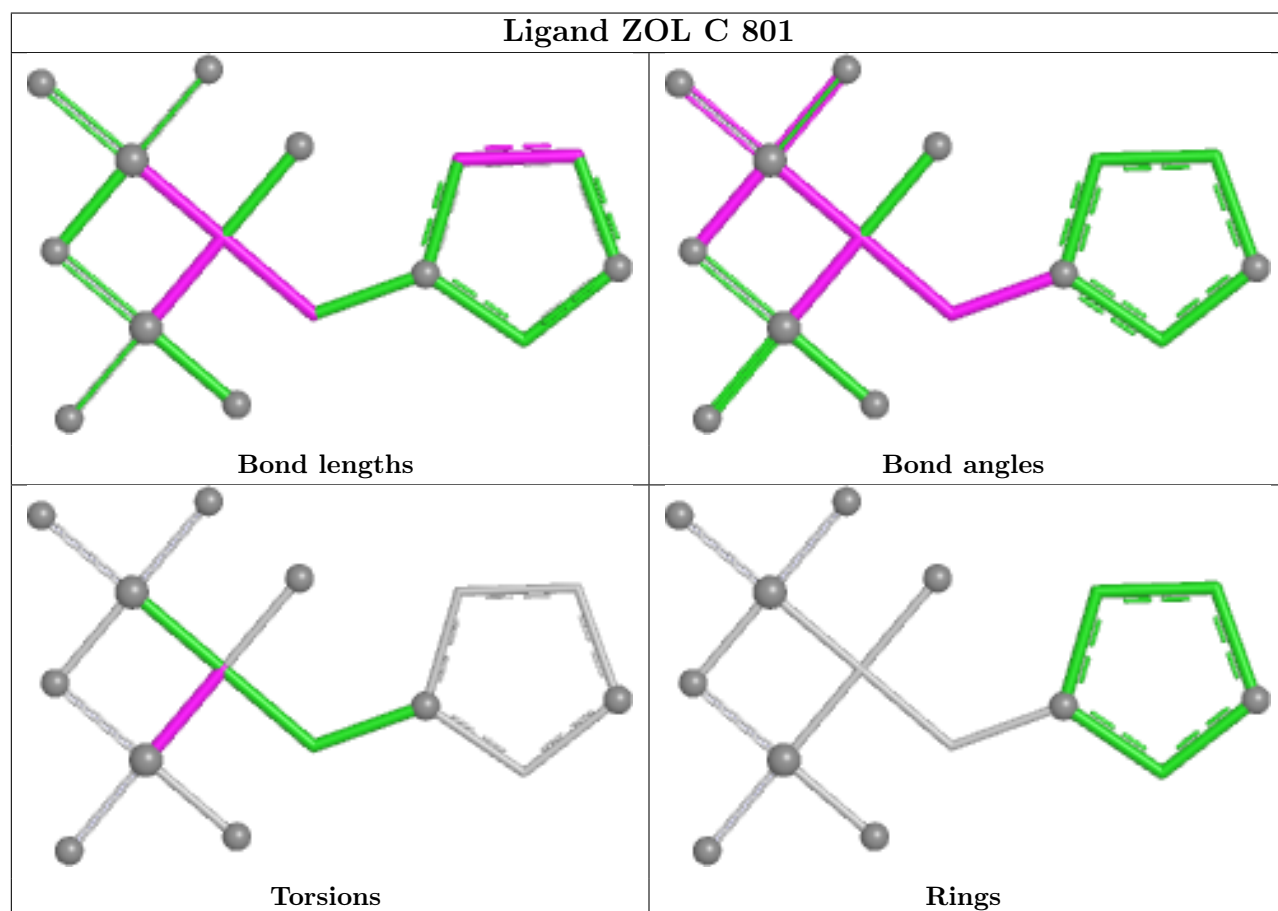
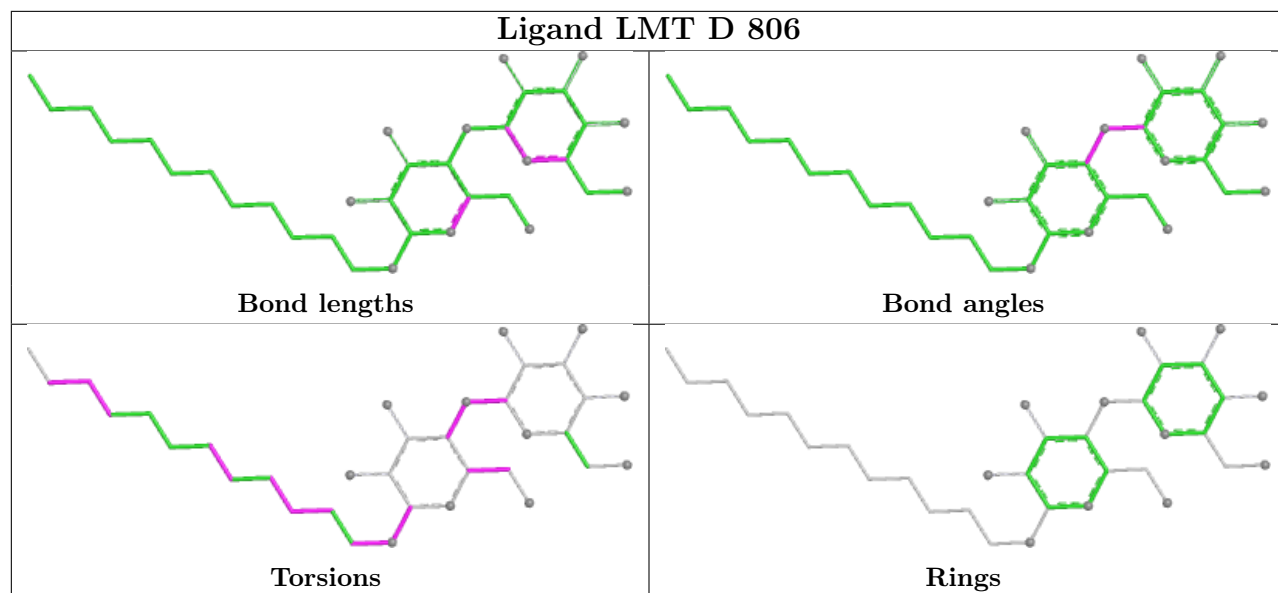
2 monomers are involved in 5 short contacts:

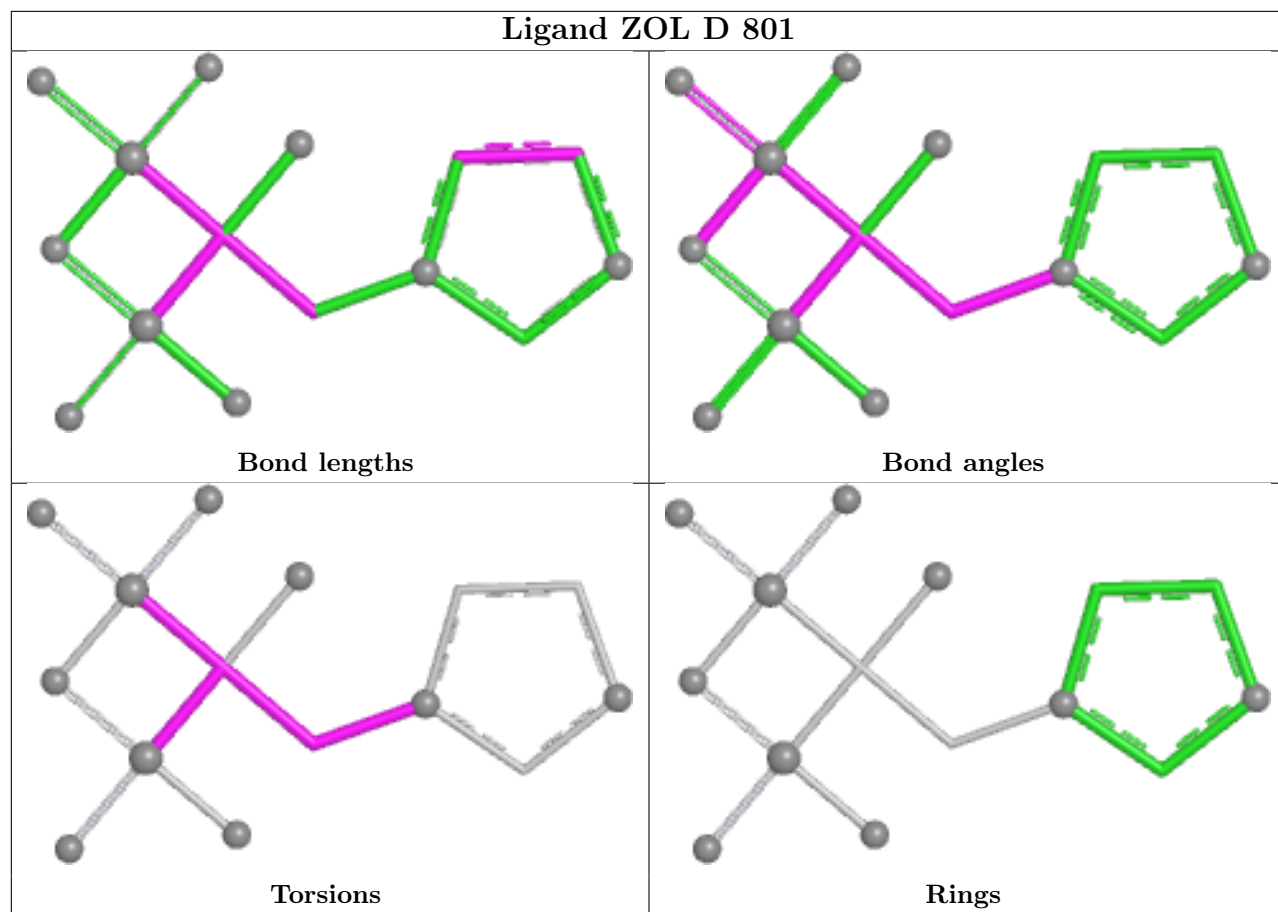
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ZOL	3	0
2	D	801	ZOL	2	0

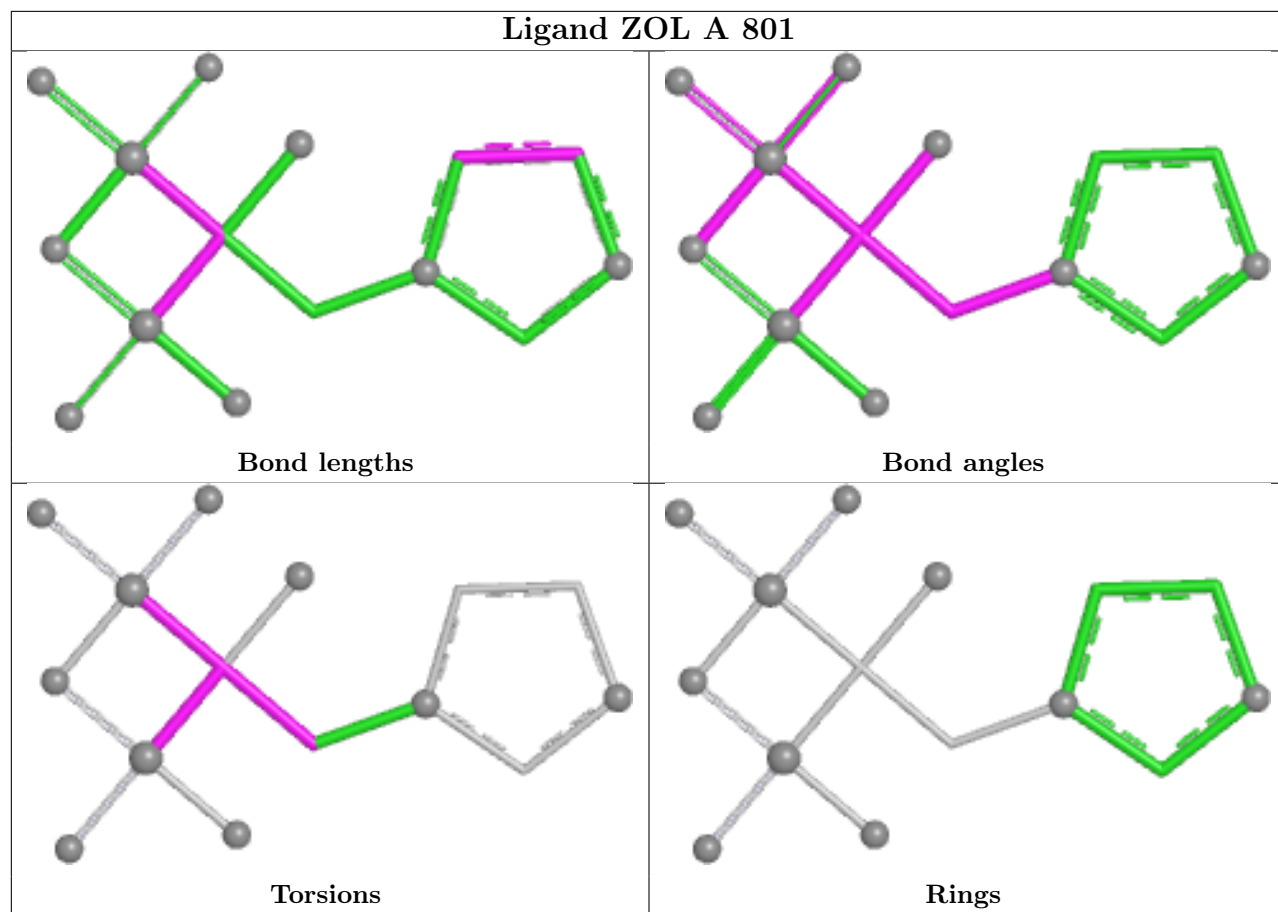
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 than 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	724/735 (98%)	0.77	85 (11%) 9 8	64, 106, 145, 175	0
1	B	716/735 (97%)	0.69	77 (10%) 11 9	62, 107, 145, 184	0
1	C	720/735 (97%)	0.66	95 (13%) 7 6	61, 106, 148, 178	0
1	D	716/735 (97%)	0.77	93 (12%) 7 6	71, 124, 167, 199	0
All	All	2876/2940 (97%)	0.72	350 (12%) 8 7	61, 110, 154, 199	0

All (350) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	THR	11.4
1	D	458	ASP	10.7
1	D	464	ALA	10.3
1	A	399	ILE	9.9
1	A	158	LEU	9.6
1	C	353	LEU	9.5
1	B	458	ASP	9.3
1	B	493	THR	9.1
1	D	454	SER	8.7
1	D	694	LEU	8.5
1	A	262	MET	8.5
1	A	535	LEU	8.3
1	B	495	ALA	8.3
1	B	496	ALA	8.0
1	C	673	GLY	7.9
1	C	240	LEU	7.6
1	D	119	LEU	7.6
1	B	460	TYR	7.3
1	D	463	ILE	7.3
1	B	9	LEU	7.3
1	C	262	MET	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	498	GLY	7.1
1	A	258	LEU	6.9
1	D	494	THR	6.7
1	B	497	ILE	6.7
1	C	669	GLY	6.7
1	A	40	SER	6.6
1	A	259	ALA	6.6
1	B	491	GLY	6.6
1	D	89	SER	6.6
1	C	352	VAL	6.5
1	D	143	LEU	6.4
1	D	652	THR	6.4
1	B	655	SER	6.4
1	A	698	VAL	6.4
1	D	240	LEU	6.2
1	B	260	SER	6.1
1	D	651	LEU	6.0
1	D	460	TYR	6.0
1	D	497	ILE	6.0
1	B	256	ILE	6.0
1	B	8	PHE	5.9
1	B	253	VAL	5.9
1	D	410	LEU	5.9
1	A	454	SER	5.8
1	D	498	GLY	5.8
1	A	519	PHE	5.8
1	C	256	ILE	5.8
1	A	263	PHE	5.7
1	B	653	ALA	5.7
1	A	674	TYR	5.7
1	C	201	ALA	5.6
1	D	244	LEU	5.6
1	C	514	PHE	5.6
1	C	458	ASP	5.5
1	C	457	VAL	5.5
1	B	12	LEU	5.5
1	B	540	LEU	5.5
1	A	490	VAL	5.4
1	A	494	THR	5.3
1	A	261	TYR	5.2
1	D	8	PHE	5.2
1	C	244	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	539	MET	5.2
1	D	437	LEU	5.1
1	A	386	TYR	5.0
1	B	102	ASN	5.0
1	C	438	TYR	4.9
1	D	98	ALA	4.9
1	A	381	GLU	4.9
1	C	670	ASN	4.9
1	D	122	ALA	4.9
1	A	697	THR	4.8
1	B	694	LEU	4.8
1	C	675	GLY	4.7
1	D	6	LEU	4.7
1	C	12	LEU	4.7
1	A	491	GLY	4.6
1	A	192	VAL	4.6
1	B	119	LEU	4.5
1	C	349	GLY	4.5
1	B	123	TYR	4.5
1	D	253	VAL	4.5
1	D	102	ASN	4.5
1	C	197	TYR	4.5
1	B	341	TYR	4.4
1	A	492	ASN	4.4
1	C	437	LEU	4.4
1	C	455	VAL	4.3
1	A	675	GLY	4.3
1	B	490	VAL	4.3
1	C	260	SER	4.3
1	C	613	TYR	4.3
1	A	157	ASN	4.3
1	C	491	GLY	4.2
1	D	451	VAL	4.2
1	A	667	GLU	4.2
1	B	652	THR	4.2
1	B	644	SER	4.1
1	A	514	PHE	4.1
1	B	657	GLY	4.1
1	C	258	LEU	4.0
1	C	488	ASP	4.0
1	D	698	VAL	4.0
1	D	696	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	459	SER	3.9
1	B	545	ILE	3.9
1	A	98	ALA	3.9
1	A	400	GLU	3.9
1	D	656	GLY	3.9
1	A	670	ASN	3.8
1	B	499	LYS	3.8
1	C	266	TYR	3.8
1	A	236	ASP	3.8
1	C	406	ILE	3.8
1	A	264	PRO	3.8
1	D	645	GLY	3.7
1	D	44	SER	3.7
1	A	325	LEU	3.7
1	D	493	THR	3.7
1	D	495	ALA	3.7
1	A	278	VAL	3.7
1	D	9	LEU	3.7
1	A	511	LEU	3.6
1	B	126	GLY	3.6
1	D	100	ARG	3.6
1	D	467	ALA	3.6
1	C	129	MET	3.5
1	B	461	GLY	3.5
1	D	690	VAL	3.5
1	C	511	LEU	3.5
1	A	322	ASN	3.5
1	C	351	ASP	3.4
1	C	460	TYR	3.4
1	D	545	ILE	3.4
1	C	236	ASP	3.4
1	C	371	PHE	3.4
1	C	459	SER	3.3
1	D	138	LEU	3.3
1	D	648	LEU	3.3
1	B	563	ILE	3.3
1	C	323	ILE	3.3
1	B	651	LEU	3.3
1	A	365	SER	3.3
1	A	95	MET	3.3
1	A	404	MET	3.3
1	B	122	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	137	ALA	3.3
1	A	534	VAL	3.3
1	C	194	GLY	3.3
1	B	317	PRO	3.2
1	A	265	ILE	3.2
1	B	522	ILE	3.2
1	B	538	ASN	3.2
1	B	374	ILE	3.2
1	D	466	ASN	3.2
1	A	165	LEU	3.2
1	D	450	PHE	3.2
1	A	406	ILE	3.2
1	C	253	VAL	3.2
1	B	101	ALA	3.2
1	A	401	GLY	3.2
1	A	353	LEU	3.2
1	A	191	ARG	3.2
1	B	649	ALA	3.2
1	C	451	VAL	3.1
1	C	486	HIS	3.1
1	B	479	GLU	3.1
1	D	257	ILE	3.1
1	A	515	ALA	3.1
1	B	656	GLY	3.1
1	C	263	PHE	3.1
1	D	249	VAL	3.1
1	A	260	SER	3.1
1	C	414	MET	3.1
1	B	254	SER	3.1
1	B	696	ASP	3.1
1	C	410	LEU	3.0
1	C	616	PHE	3.0
1	C	674	TYR	3.0
1	A	443	ALA	3.0
1	B	431	ALA	3.0
1	A	600	ILE	3.0
1	B	537	LEU	2.9
1	A	207	LEU	2.9
1	A	701	SER	2.9
1	D	93	VAL	2.9
1	D	618	ALA	2.9
1	C	678	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	491	GLY	2.9
1	D	258	LEU	2.9
1	A	366	ALA	2.9
1	C	259	ALA	2.9
1	B	234	VAL	2.9
1	D	103	VAL	2.8
1	A	235	GLY	2.8
1	B	398	SER	2.8
1	C	25	VAL	2.8
1	B	244	LEU	2.8
1	B	463	ILE	2.8
1	D	92	ILE	2.8
1	D	414	MET	2.8
1	A	266	TYR	2.8
1	C	250	GLY	2.8
1	C	13	VAL	2.8
1	A	437	LEU	2.8
1	A	457	VAL	2.8
1	C	642	VAL	2.8
1	D	462	PRO	2.8
1	A	489	ALA	2.7
1	C	123	TYR	2.7
1	C	386	TYR	2.7
1	D	248	PHE	2.7
1	D	126	GLY	2.7
1	C	77	GLY	2.7
1	D	123	TYR	2.7
1	A	681	HIS	2.7
1	B	501	PHE	2.7
1	A	9	LEU	2.7
1	D	619	ILE	2.6
1	A	516	SER	2.6
1	C	512	SER	2.6
1	C	584	ILE	2.6
1	B	654	ASN	2.6
1	A	340	THR	2.6
1	A	666	LEU	2.6
1	D	353	LEU	2.6
1	D	620	LEU	2.6
1	D	702	LEU	2.6
1	D	539	MET	2.6
1	B	455	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	698	VAL	2.6
1	A	699	GLY	2.6
1	B	401	GLY	2.6
1	B	410	LEU	2.6
1	D	196	VAL	2.6
1	C	379	TRP	2.5
1	C	677	GLY	2.5
1	B	190	ASP	2.5
1	C	127	SER	2.5
1	D	105	VAL	2.5
1	C	322	ASN	2.5
1	C	495	ALA	2.5
1	C	28	LYS	2.5
1	D	563	ILE	2.5
1	B	6	LEU	2.5
1	B	684	LEU	2.5
1	B	500	GLY	2.5
1	D	260	SER	2.5
1	D	659	TRP	2.5
1	D	689	THR	2.5
1	A	531	PRO	2.5
1	A	676	LYS	2.4
1	C	513	LEU	2.4
1	A	694	LEU	2.4
1	D	438	TYR	2.4
1	C	510	ALA	2.4
1	A	525	SER	2.4
1	C	537	LEU	2.4
1	C	235	GLY	2.4
1	D	109	ALA	2.4
1	A	558	PHE	2.4
1	C	376	ILE	2.4
1	A	512	SER	2.4
1	C	83	GLY	2.3
1	B	2	TYR	2.3
1	C	665	TYR	2.3
1	D	496	ALA	2.3
1	D	262	MET	2.3
1	B	533	LEU	2.3
1	C	390	PRO	2.3
1	C	54	THR	2.3
1	D	327	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	668	ALA	2.3
1	B	618	ALA	2.3
1	D	615	ALA	2.3
1	A	159	ASN	2.3
1	A	458	ASP	2.3
1	A	67	LEU	2.3
1	D	519	PHE	2.3
1	C	239	GLY	2.3
1	B	449	SER	2.3
1	C	355	PHE	2.3
1	B	406	ILE	2.3
1	C	29	PRO	2.3
1	C	200	ALA	2.3
1	B	384	THR	2.3
1	D	321	LEU	2.3
1	B	100	ARG	2.3
1	C	321	LEU	2.2
1	C	487	LEU	2.2
1	B	559	SER	2.2
1	D	655	SER	2.2
1	A	239	GLY	2.2
1	B	194	GLY	2.2
1	C	84	ALA	2.2
1	C	326	TRP	2.2
1	D	169	PHE	2.2
1	C	73	THR	2.2
1	B	451	VAL	2.2
1	A	360	ILE	2.2
1	D	173	ALA	2.2
1	D	461	GLY	2.2
1	D	584	ILE	2.2
1	A	631	ALA	2.2
1	C	696	ASP	2.2
1	A	402	THR	2.2
1	B	454	SER	2.2
1	C	456	SER	2.2
1	C	204	ALA	2.2
1	B	488	ASP	2.2
1	D	263	PHE	2.2
1	B	723	VAL	2.1
1	A	179	TYR	2.1
1	B	255	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	559	SER	2.1
1	A	71	PHE	2.1
1	A	414	MET	2.1
1	B	56	ALA	2.1
1	D	65	ALA	2.1
1	D	106	ALA	2.1
1	C	667	GLU	2.1
1	C	133	VAL	2.1
1	C	432	ASP	2.1
1	D	455	VAL	2.1
1	A	424	LEU	2.1
1	C	305	ILE	2.1
1	D	406	ILE	2.1
1	C	268	GLN	2.1
1	A	361	SER	2.1
1	A	321	LEU	2.1
1	D	377	GLY	2.1
1	D	675	GLY	2.1
1	C	450	PHE	2.1
1	C	234	VAL	2.1
1	D	490	VAL	2.1
1	C	676	LYS	2.1
1	D	286	LEU	2.1
1	C	41	TYR	2.1
1	C	482	LYS	2.0
1	A	644	SER	2.0
1	A	240	LEU	2.0
1	A	639	ILE	2.0
1	C	65	ALA	2.0
1	C	612	GLY	2.0
1	D	723	VAL	2.0
1	B	327	THR	2.0
1	D	673	GLY	2.0
1	D	540	LEU	2.0
1	B	257	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

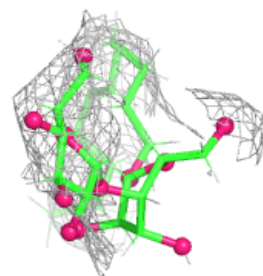
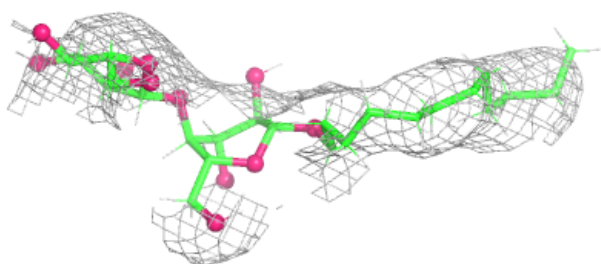
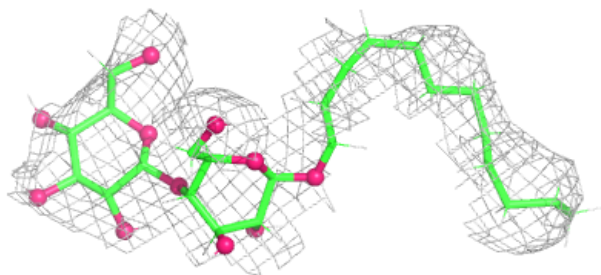
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LMT	D	806	35/35	0.28	0.12	118,166,195,204	0
3	MG	B	802	1/1	0.33	0.20	110,110,110,110	0
3	MG	C	803	1/1	0.63	0.17	116,116,116,116	0
3	MG	B	805	1/1	0.81	0.19	122,122,122,122	0
3	MG	C	804	1/1	0.83	0.17	119,119,119,119	0
3	MG	D	803	1/1	0.84	0.15	132,132,132,132	0
3	MG	C	802	1/1	0.89	0.21	104,104,104,104	0
3	MG	B	804	1/1	0.90	0.12	98,98,98,98	0
3	MG	A	804	1/1	0.91	0.20	86,86,86,86	0
3	MG	A	805	1/1	0.92	0.17	115,115,115,115	0
2	ZOL	C	801	16/16	0.93	0.11	107,146,179,184	0
2	ZOL	D	801	16/16	0.93	0.11	131,151,178,183	0
2	ZOL	A	801	16/16	0.93	0.10	101,123,146,159	0
2	ZOL	B	801	16/16	0.93	0.09	108,130,157,168	0
3	MG	D	805	1/1	0.94	0.12	133,133,133,133	0
3	MG	D	804	1/1	0.96	0.15	127,127,127,127	0
3	MG	A	803	1/1	0.97	0.09	101,101,101,101	0
3	MG	C	805	1/1	0.97	0.10	131,131,131,131	0
3	MG	B	803	1/1	0.97	0.11	111,111,111,111	0
3	MG	A	802	1/1	0.98	0.15	92,92,92,92	0
3	MG	D	802	1/1	0.98	0.12	138,138,138,138	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.

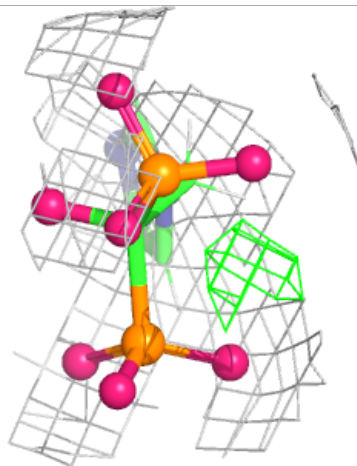
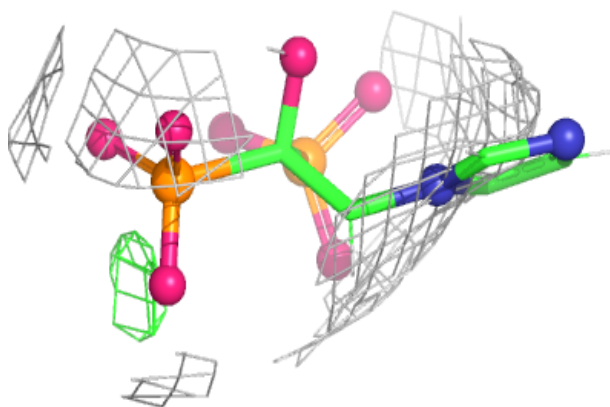
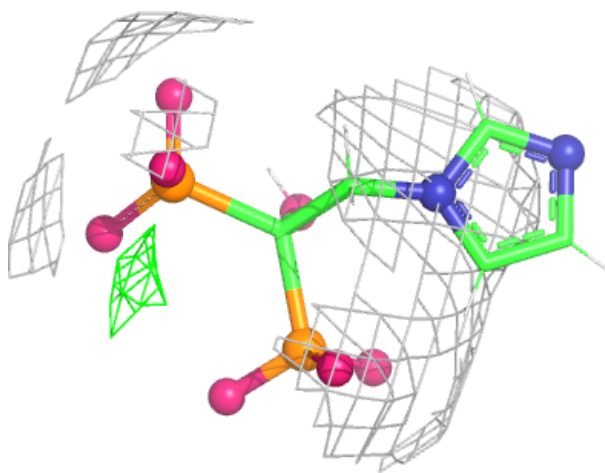
Electron density around LMT D 806:

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



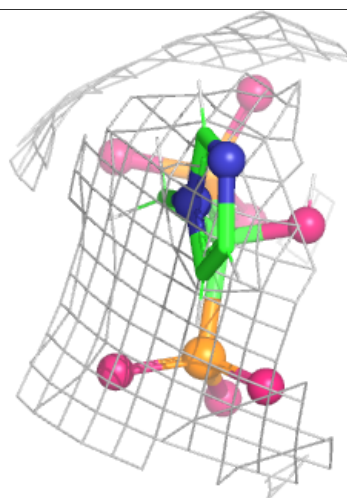
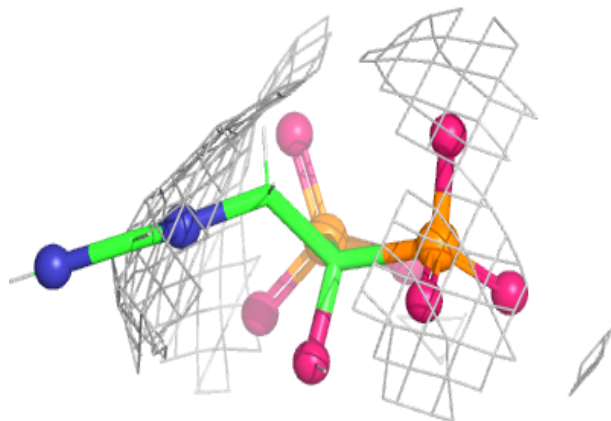
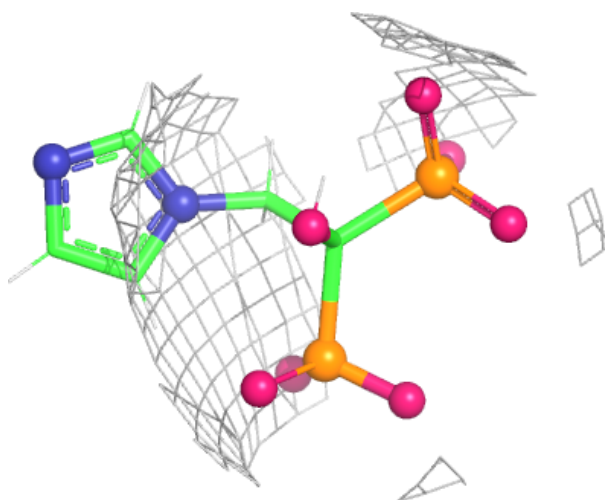
Electron density around ZOL C 801:

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



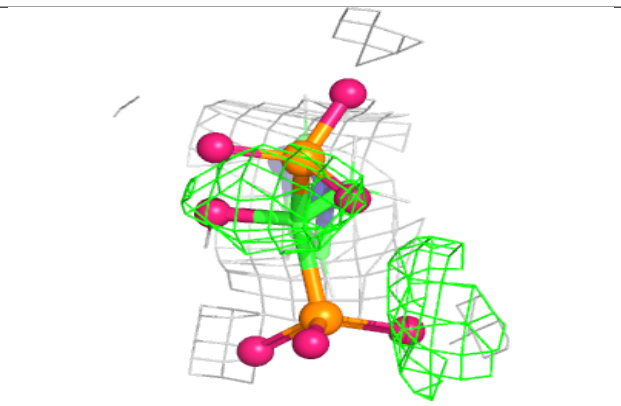
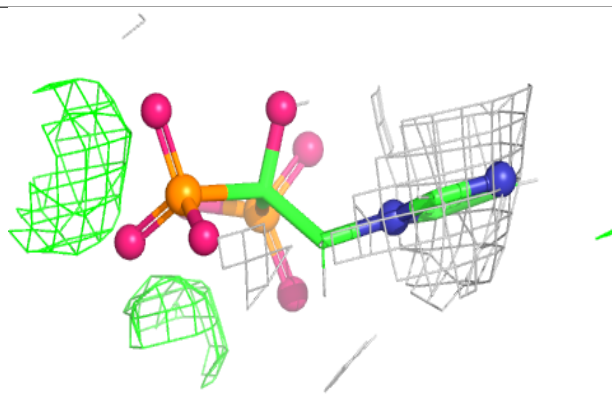
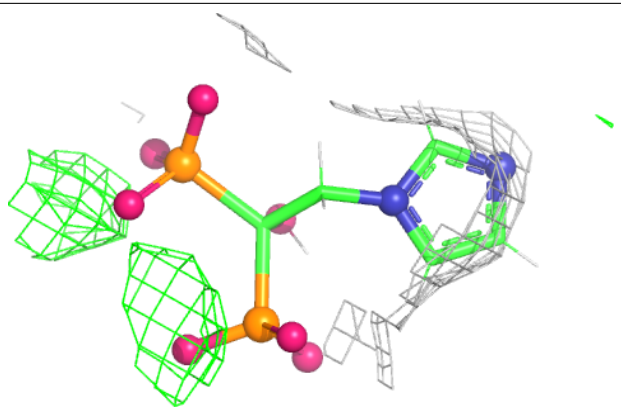
Electron density around ZOL D 801:

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

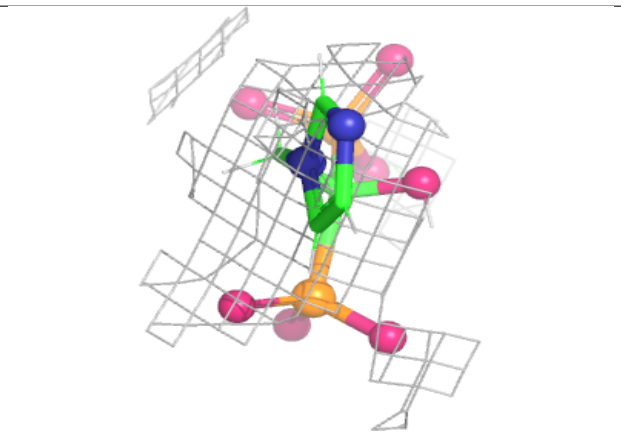
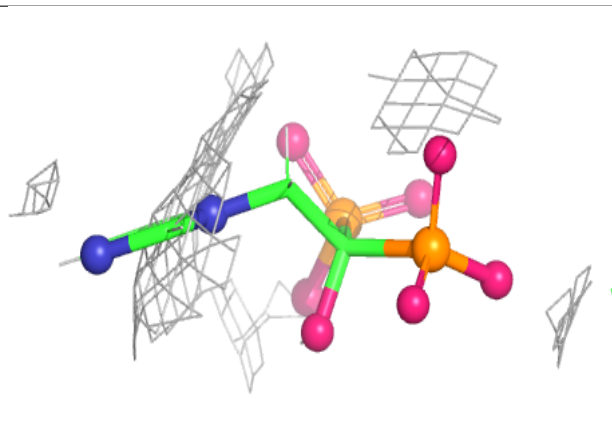
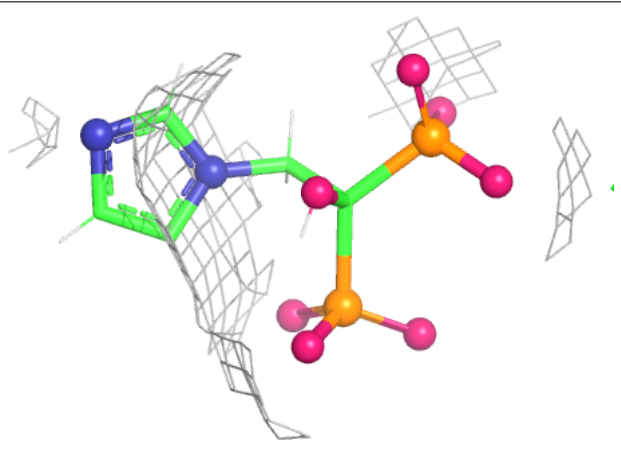


Electron density around ZOL A 801:

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

**Electron density around ZOL B 801:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.