



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:54 PM UTC

PDB ID : 6KQY / pdb_00006kqy
Title : Crystal structure of human leucyl-tRNA synthetase, Leucine-bound form
Authors : Kim, S.; Son, J.; Kim, S.; Hwang, K.Y.
Deposited on : 2019-08-20
Resolution : 3.30 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

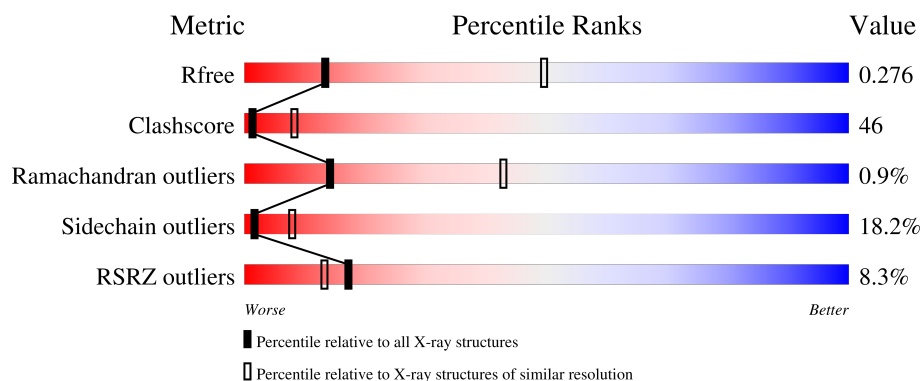
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	1188	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

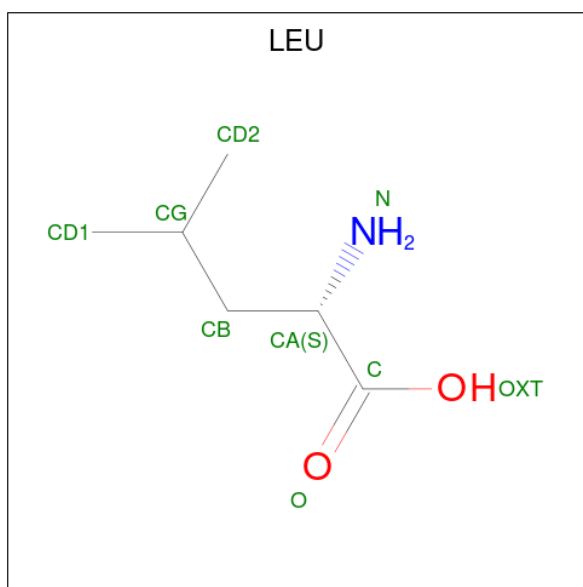
- Molecule 1 is a protein called Leucine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1002	Total	C	N	O	S	0	0	0
			8088	5204	1343	1488	53			

There are 12 discrepancies between the modelled and reference sequences:

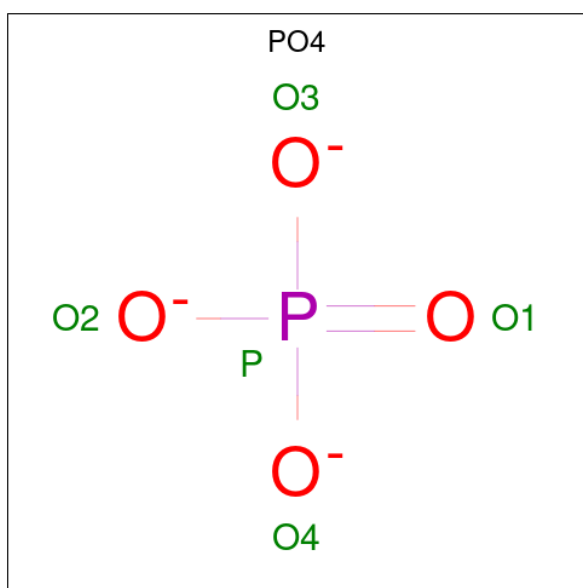
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9P2J5
A	-10	ARG	-	expression tag	UNP Q9P2J5
A	-9	GLY	-	expression tag	UNP Q9P2J5
A	-8	SER	-	expression tag	UNP Q9P2J5
A	-7	HIS	-	expression tag	UNP Q9P2J5
A	-6	HIS	-	expression tag	UNP Q9P2J5
A	-5	HIS	-	expression tag	UNP Q9P2J5
A	-4	HIS	-	expression tag	UNP Q9P2J5
A	-3	HIS	-	expression tag	UNP Q9P2J5
A	-2	HIS	-	expression tag	UNP Q9P2J5
A	-1	GLY	-	expression tag	UNP Q9P2J5
A	0	SER	-	expression tag	UNP Q9P2J5

- Molecule 2 is LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	447	Total 447	O 447	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.74Å 123.74Å 536.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.76 – 3.30 49.76 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.76-3.30) 97.9 (49.76-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.251 , 0.276 0.250 , 0.276	Depositor DCC
R_{free} test set	1937 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	8558	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.57	0/8288	0.90	14/11203 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	971	VAL	N-CA-C	-9.37	101.26	110.72
1	A	949	HIS	CA-C-N	8.10	131.48	120.54
1	A	949	HIS	C-N-CA	8.10	131.48	120.54
1	A	949	HIS	O-C-N	7.27	129.86	122.08
1	A	516	SER	O-C-N	6.76	129.03	122.07
1	A	52	TYR	CA-CB-CG	6.34	125.32	113.90
1	A	951	THR	CB-CA-C	-6.11	101.56	110.96
1	A	368	SER	N-CA-C	-5.82	106.52	113.21
1	A	516	SER	CA-C-N	5.55	132.14	121.54
1	A	516	SER	C-N-CA	5.55	132.14	121.54
1	A	517	ARG	N-CA-C	-5.40	99.30	110.80
1	A	956	ARG	N-CA-C	-5.39	105.30	111.07
1	A	1041	ALA	CB-CA-C	5.19	118.81	111.86
1	A	1043	GLU	N-CA-C	-5.08	106.33	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8088	0	8046	747	6
2	A	18	0	20	4	0
3	A	5	0	0	0	0
4	A	447	0	0	77	0
All	All	8558	0	8066	747	6

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 46.

All (747) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:CYS:CB	1:A:451:ILE:HD12	1.49	1.42
1:A:958:HIS:HE1	1:A:962:ASN:ND2	1.06	1.42
1:A:958:HIS:CE1	1:A:962:ASN:ND2	1.87	1.39
1:A:446:CYS:CB	1:A:451:ILE:CD1	2.08	1.22
1:A:958:HIS:CE1	1:A:962:ASN:HD22	1.55	1.19
1:A:446:CYS:SG	1:A:451:ILE:HD11	0.75	1.15
1:A:446:CYS:SG	1:A:451:ILE:CD1	1.06	1.13
1:A:446:CYS:HB3	1:A:451:ILE:HD12	1.31	1.09
1:A:951:THR:CG2	1:A:989:VAL:HG13	1.83	1.08
1:A:945:PRO:HD2	1:A:948:GLN:CB	1.83	1.08
1:A:205:PHE:HB3	1:A:611:GLN:HE22	1.13	1.08
1:A:516:SER:OG	4:A:1301:HOH:O	1.62	1.05
1:A:945:PRO:HD2	1:A:948:GLN:HB2	1.03	1.03
1:A:945:PRO:CD	1:A:948:GLN:HB2	1.90	1.02
1:A:603:PHE:CZ	1:A:611:GLN:OE1	2.14	1.01
1:A:446:CYS:SG	1:A:451:ILE:CG1	2.51	0.98
1:A:517:ARG:HD3	4:A:1301:HOH:O	1.67	0.94
1:A:951:THR:CG2	1:A:989:VAL:CG1	2.46	0.94
1:A:951:THR:HG21	1:A:989:VAL:HG13	1.48	0.93
1:A:939:TYR:HB3	1:A:1041:ALA:HB2	1.49	0.92
1:A:48:VAL:HG21	1:A:74:VAL:HG11	1.51	0.91
1:A:970:LYS:CE	1:A:970:LYS:HA	2.02	0.90
1:A:452:GLN:HB3	4:A:1485:HOH:O	1.70	0.90
1:A:603:PHE:CE2	1:A:611:GLN:OE1	2.25	0.90
1:A:951:THR:HG23	1:A:989:VAL:CG1	2.01	0.89
1:A:352:LEU:HD11	1:A:357:ILE:HD11	1.55	0.88
1:A:308:ARG:NH1	1:A:378:LEU:O	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LEU:HD13	1:A:654:LYS:HB3	1.56	0.88
1:A:956:ARG:HG2	1:A:1008:LEU:CD2	2.02	0.87
1:A:970:LYS:HA	1:A:970:LYS:HE2	1.56	0.87
1:A:174:PHE:HB3	1:A:180:TRP:HE1	1.36	0.87
1:A:958:HIS:CE1	1:A:962:ASN:CG	2.51	0.87
1:A:599:ILE:HA	1:A:689:HIS:HE1	1.39	0.86
1:A:652:LYS:HA	1:A:655:LEU:HD12	1.56	0.86
1:A:409:LYS:H	1:A:409:LYS:HZ2	1.24	0.84
1:A:811:ASN:HB2	1:A:820:ALA:HB2	1.57	0.84
1:A:952:LEU:O	1:A:956:ARG:HG3	1.79	0.83
1:A:488:GLN:NE2	4:A:1309:HOH:O	2.11	0.83
1:A:51:PRO:HG2	1:A:673:SER:HB2	1.62	0.82
1:A:239:ILE:HD12	1:A:239:ILE:H	1.45	0.81
1:A:944:TYR:HB3	1:A:949:HIS:HB3	1.61	0.81
1:A:308:ARG:HB3	1:A:311:MET:HE3	1.64	0.80
1:A:1019:VAL:O	1:A:1023:ASN:ND2	2.13	0.80
1:A:446:CYS:SG	1:A:451:ILE:HD12	1.39	0.80
1:A:533:ASP:N	4:A:1312:HOH:O	2.12	0.80
1:A:384:LYS:HZ1	2:A:1202:LEU:HD21	1.47	0.79
1:A:693:TRP:HD1	1:A:696:GLN:HG3	1.48	0.79
1:A:435:PRO:HD2	1:A:474:GLU:HG2	1.64	0.78
1:A:446:CYS:HG	1:A:451:ILE:CD1	0.95	0.78
1:A:446:CYS:CB	1:A:451:ILE:HD11	1.95	0.78
1:A:405:ASP:O	1:A:409:LYS:NZ	2.17	0.78
1:A:217:PHE:HE2	1:A:600:TYR:HA	1.49	0.77
1:A:951:THR:HG23	1:A:989:VAL:HG13	1.64	0.77
1:A:347:PRO:HG2	4:A:1313:HOH:O	1.85	0.76
1:A:599:ILE:HA	1:A:689:HIS:CE1	2.20	0.76
1:A:949:HIS:CD2	1:A:949:HIS:H	2.02	0.76
1:A:508:MET:HB3	1:A:523:VAL:HG11	1.66	0.76
1:A:583:LEU:HD23	1:A:584:PRO:HD2	1.65	0.76
1:A:1030:SER:N	4:A:1317:HOH:O	2.16	0.76
1:A:1035:HIS:O	4:A:1303:HOH:O	2.03	0.75
1:A:105:LYS:HB3	1:A:175:SER:HB3	1.67	0.75
1:A:718:SER:O	1:A:721:THR:OG1	2.04	0.75
1:A:962:ASN:HD21	1:A:966:LEU:HD23	1.51	0.75
1:A:951:THR:HG23	1:A:989:VAL:HG11	1.67	0.75
1:A:230:LYS:HZ2	1:A:539:TRP:CG	2.05	0.74
1:A:456:ASP:HB3	1:A:459:LYS:HB2	1.68	0.74
1:A:249:MET:O	1:A:253:ARG:NE	2.20	0.74
1:A:404:ARG:HB3	1:A:408:LYS:HZ1	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:HB2	1:A:817:PHE:CE2	2.21	0.74
1:A:513:GLN:N	4:A:1322:HOH:O	2.19	0.74
1:A:355:GLU:OE1	4:A:1305:HOH:O	2.05	0.74
1:A:632:LYS:NZ	1:A:636:ASP:OD2	2.21	0.73
1:A:689:HIS:HD2	1:A:701:PRO:HG3	1.54	0.73
1:A:550:LEU:HD21	1:A:704:VAL:HG23	1.69	0.73
1:A:363:SER:HA	1:A:370:LYS:O	1.88	0.73
1:A:287:ILE:HG23	1:A:323:ILE:HB	1.70	0.73
1:A:95:MET:O	1:A:98:LYS:N	2.22	0.72
1:A:834:LYS:HA	1:A:837:GLU:HB2	1.70	0.72
1:A:808:THR:HG21	1:A:858:LEU:HD13	1.72	0.72
1:A:956:ARG:CG	1:A:1008:LEU:CD2	2.66	0.72
1:A:408:LYS:HB2	1:A:409:LYS:HZ2	1.55	0.72
1:A:295:ARG:O	1:A:298:THR:OG1	2.08	0.71
1:A:158:TRP:N	4:A:1325:HOH:O	2.21	0.71
1:A:956:ARG:HG2	1:A:1008:LEU:HD22	1.71	0.71
1:A:445:ILE:HD13	1:A:466:LYS:HD2	1.72	0.71
1:A:1020:LEU:C	1:A:1022:GLU:H	1.97	0.71
1:A:969:ASN:HA	1:A:972:ILE:HG13	1.73	0.71
1:A:272:LEU:HD11	1:A:363:SER:HB2	1.71	0.71
1:A:276:PRO:HD2	1:A:279:LEU:HD12	1.72	0.71
1:A:1057:PRO:O	4:A:1306:HOH:O	2.09	0.71
1:A:962:ASN:ND2	1:A:965:LYS:O	2.24	0.70
1:A:956:ARG:NH1	1:A:1010:LEU:HD22	2.07	0.70
1:A:298:THR:HB	1:A:392:VAL:HG11	1.74	0.70
1:A:852:ILE:HD11	1:A:874:LEU:HD11	1.73	0.70
1:A:236:ARG:HB2	1:A:529:GLN:OE1	1.91	0.70
1:A:405:ASP:HA	1:A:408:LYS:HD2	1.73	0.70
1:A:429:VAL:HG12	1:A:431:VAL:HG13	1.74	0.70
1:A:601:MET:HE2	1:A:671:ARG:NH1	2.06	0.70
1:A:85:LEU:HG	1:A:87:PRO:HD3	1.75	0.69
1:A:397:PRO:HB2	1:A:463:ALA:HB1	1.73	0.69
1:A:24:TRP:CH2	1:A:864:PRO:HB2	2.28	0.69
1:A:384:LYS:NZ	2:A:1202:LEU:HD21	2.07	0.69
1:A:594:LEU:HD13	1:A:684:TYR:HE2	1.58	0.69
1:A:97:ILE:O	4:A:1311:HOH:O	2.11	0.69
1:A:629:GLN:OE1	4:A:1310:HOH:O	2.11	0.68
1:A:194:ARG:NH1	1:A:732:ASP:OD1	2.22	0.68
1:A:635:TRP:HA	1:A:638:VAL:HG12	1.74	0.68
1:A:908:ASP:O	4:A:1307:HOH:O	2.10	0.68
1:A:93:THR:HG22	1:A:94:GLY:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:HIS:HE1	1:A:962:ASN:HD22	0.69	0.68
1:A:217:PHE:HA	4:A:1377:HOH:O	1.94	0.68
1:A:252:ASP:O	1:A:516:SER:O	2.12	0.68
1:A:414:ALA:O	4:A:1308:HOH:O	2.10	0.68
1:A:405:ASP:CG	1:A:454:GLN:HB2	2.18	0.68
1:A:47:PHE:HD2	1:A:668:VAL:HA	1.59	0.68
1:A:24:TRP:HH2	1:A:864:PRO:HB2	1.60	0.67
1:A:667:PRO:HB3	1:A:699:LYS:HA	1.76	0.67
1:A:191:ASP:HB3	1:A:727:LEU:HD23	1.75	0.67
1:A:540:LYS:NZ	1:A:565:LEU:O	2.28	0.67
1:A:638:VAL:O	1:A:659:LYS:NZ	2.18	0.67
1:A:50:PHE:HD2	1:A:88:PHE:HE1	1.40	0.67
1:A:69:LYS:HE3	1:A:705:ARG:HH21	1.60	0.67
1:A:567:TRP:O	1:A:569:GLN:NE2	2.28	0.67
1:A:1043:GLU:O	1:A:1043:GLU:HG2	1.95	0.67
1:A:633:GLU:HA	1:A:636:ASP:HB2	1.77	0.67
1:A:735:SER:O	1:A:738:GLY:N	2.28	0.66
1:A:317:GLU:O	4:A:1313:HOH:O	2.12	0.66
1:A:408:LYS:HB2	1:A:409:LYS:NZ	2.09	0.66
1:A:518:SER:N	4:A:1301:HOH:O	2.25	0.66
1:A:600:TYR:OH	1:A:671:ARG:NH2	2.26	0.66
1:A:106:ARG:HA	1:A:109:GLU:HB2	1.77	0.66
1:A:328:GLN:NE2	4:A:1330:HOH:O	2.23	0.66
1:A:784:LEU:HD13	1:A:845:ARG:HB3	1.76	0.66
1:A:819:GLU:OE1	4:A:1315:HOH:O	2.14	0.66
1:A:405:ASP:HB2	1:A:454:GLN:HE21	1.59	0.66
1:A:796:VAL:HA	1:A:895:LEU:HD23	1.77	0.66
1:A:812:TYR:HE2	1:A:861:PRO:HG3	1.61	0.66
1:A:293:THR:HG1	2:A:1202:LEU:N	1.94	0.66
1:A:306:TRP:HB2	1:A:389:VAL:HG23	1.76	0.66
1:A:982:LEU:HD11	1:A:989:VAL:HG21	1.77	0.66
1:A:266:LEU:HD21	1:A:290:VAL:HB	1.78	0.66
1:A:55:MET:HA	1:A:55:MET:HE2	1.78	0.65
1:A:607:ALA:O	1:A:611:GLN:CG	2.45	0.65
1:A:466:LYS:C	1:A:468:TYR:H	2.04	0.65
1:A:624:GLY:O	4:A:1314:HOH:O	2.14	0.65
1:A:195:MET:HG2	1:A:197:LEU:HD21	1.78	0.65
1:A:844:HIS:CE1	1:A:846:GLU:HB2	2.30	0.65
1:A:166:LEU:HB2	1:A:171:ILE:HG12	1.78	0.65
1:A:625:ILE:HG12	1:A:650:ILE:HD13	1.78	0.65
1:A:539:TRP:CZ2	1:A:691:ALA:HB2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ILE:HG12	1:A:739:MET:HE1	1.79	0.65
1:A:113:CYS:HB2	4:A:1353:HOH:O	1.96	0.65
1:A:404:ARG:NH1	4:A:1338:HOH:O	2.28	0.65
1:A:445:ILE:HB	1:A:466:LYS:HD2	1.79	0.64
1:A:405:ASP:HB2	1:A:454:GLN:NE2	2.12	0.64
1:A:1044:ALA:O	4:A:1316:HOH:O	2.15	0.64
1:A:731:ILE:HG12	1:A:739:MET:CE	2.26	0.64
1:A:761:ASP:O	1:A:764:ILE:HG12	1.98	0.64
1:A:693:TRP:HB3	1:A:696:GLN:HB2	1.80	0.64
1:A:446:CYS:SG	1:A:451:ILE:HD13	1.35	0.64
1:A:736:ALA:O	1:A:740:ARG:HG3	1.96	0.64
1:A:798:ALA:HB2	1:A:847:LEU:HD13	1.79	0.63
1:A:469:LEU:O	1:A:472:PHE:CB	2.46	0.63
1:A:55:MET:HG2	1:A:90:LEU:HD22	1.79	0.63
1:A:207:THR:HG22	1:A:214:TYR:CE2	2.33	0.63
1:A:742:ALA:HB2	1:A:760:ALA:HB2	1.80	0.63
1:A:51:PRO:HG2	1:A:673:SER:CB	2.29	0.63
1:A:241:SER:HB3	1:A:244:ASP:HB2	1.80	0.62
1:A:581:THR:HB	1:A:591:ILE:HD12	1.80	0.62
1:A:1028:THR:HA	4:A:1384:HOH:O	1.98	0.62
1:A:700:TRP:N	4:A:1339:HOH:O	2.28	0.62
1:A:222:PHE:HE2	1:A:591:ILE:HD13	1.65	0.62
1:A:607:ALA:O	1:A:611:GLN:HG2	1.99	0.62
1:A:221:GLN:HB2	1:A:599:ILE:HD11	1.81	0.62
1:A:1003:MET:SD	1:A:1006:ARG:HD2	2.39	0.62
1:A:50:PHE:CD1	1:A:51:PRO:HD2	2.35	0.62
1:A:205:PHE:HA	1:A:615:LEU:HA	1.80	0.62
1:A:974:SER:O	1:A:978:SER:HB3	1.99	0.62
1:A:18:LYS:HE2	4:A:1343:HOH:O	1.98	0.62
1:A:545:GLN:HA	1:A:545:GLN:OE1	1.98	0.62
1:A:910:ARG:NH2	4:A:1302:HOH:O	1.99	0.62
1:A:72:PHE:CE2	1:A:744:ALA:HB2	2.34	0.62
1:A:240:TYR:HB3	1:A:524:VAL:HG13	1.82	0.62
1:A:942:LYS:NZ	1:A:943:ASN:HB2	2.14	0.61
1:A:10:VAL:HG22	1:A:764:ILE:HD12	1.83	0.61
1:A:300:PHE:HB2	1:A:431:VAL:HG11	1.82	0.61
1:A:937:THR:C	1:A:938:ILE:HD13	2.25	0.61
1:A:446:CYS:HG	1:A:451:ILE:HD13	0.46	0.61
1:A:802:ASN:HA	1:A:805:ILE:HG22	1.82	0.61
1:A:235:LYS:NZ	4:A:1346:HOH:O	2.32	0.61
1:A:269:LEU:HB3	1:A:362:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:MET:HE1	1:A:390:THR:HB	1.82	0.61
1:A:95:MET:O	1:A:97:ILE:N	2.33	0.61
1:A:856:THR:OG1	1:A:870:ILE:HG21	2.01	0.60
1:A:34:ALA:O	1:A:660:GLN:NE2	2.30	0.60
1:A:393:PRO:HB2	1:A:428:PRO:HG3	1.84	0.60
1:A:767:LEU:HD22	1:A:866:LEU:HD13	1.82	0.60
1:A:204:SER:O	1:A:611:GLN:NE2	2.34	0.60
1:A:369:TYR:HB3	1:A:372:ILE:CG2	2.31	0.60
1:A:25:ASP:OD1	4:A:1320:HOH:O	2.17	0.60
1:A:213:TYR:CZ	1:A:627:PRO:HG3	2.36	0.60
1:A:933:PRO:O	4:A:1318:HOH:O	2.16	0.60
1:A:415:LYS:HG2	1:A:416:TYR:CE2	2.36	0.60
1:A:435:PRO:HD2	1:A:474:GLU:CG	2.30	0.60
1:A:61:LEU:HA	1:A:64:THR:HG23	1.82	0.60
1:A:689:HIS:CD2	1:A:701:PRO:HG3	2.35	0.60
1:A:968:ASP:HB2	1:A:971:VAL:H	1.66	0.60
1:A:71:GLU:OE2	1:A:198:LYS:HE3	2.02	0.59
1:A:440:LEU:HD23	1:A:440:LEU:H	1.65	0.59
1:A:1012:LEU:HD21	4:A:1375:HOH:O	2.02	0.59
1:A:414:ALA:HA	1:A:418:ILE:HB	1.84	0.59
1:A:22:GLN:O	1:A:26:THR:OG1	2.19	0.59
1:A:1020:LEU:O	1:A:1022:GLU:N	2.35	0.59
1:A:202:ARG:O	1:A:608:HIS:HA	2.01	0.59
1:A:337:GLN:HA	1:A:525:ALA:H	1.68	0.59
1:A:409:LYS:HZ2	1:A:409:LYS:N	1.98	0.59
1:A:404:ARG:NE	4:A:1348:HOH:O	2.34	0.59
1:A:782:ASP:OD1	1:A:782:ASP:N	2.34	0.59
1:A:773:TRP:CZ2	1:A:832:LYS:HD2	2.36	0.59
1:A:449:LEU:O	1:A:459:LYS:NZ	2.36	0.59
1:A:848:VAL:O	1:A:852:ILE:HG23	2.02	0.59
1:A:568:LEU:HD21	1:A:684:TYR:HE1	1.68	0.59
1:A:844:HIS:HE1	1:A:846:GLU:HB2	1.68	0.59
1:A:958:HIS:CE1	1:A:962:ASN:CB	2.85	0.58
1:A:315:GLY:HA2	1:A:324:PHE:O	2.03	0.58
1:A:431:VAL:HA	4:A:1471:HOH:O	2.04	0.58
1:A:575:ARG:HG2	1:A:592:GLU:HB3	1.86	0.58
1:A:413:ARG:HH11	1:A:424:LEU:HD21	1.69	0.58
1:A:301:GLY:HA2	1:A:429:VAL:HB	1.86	0.58
1:A:470:LYS:N	4:A:1351:HOH:O	2.37	0.58
1:A:764:ILE:HA	1:A:767:LEU:HD12	1.85	0.58
1:A:69:LYS:NZ	1:A:748:ASP:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:914:LYS:O	4:A:1319:HOH:O	2.17	0.57
1:A:938:ILE:HD12	1:A:1059:ASN:HB3	1.86	0.57
1:A:95:MET:SD	1:A:246:GLN:NE2	2.77	0.57
1:A:398:ASP:OD1	1:A:399:ASP:N	2.36	0.57
1:A:47:PHE:CD2	1:A:668:VAL:HA	2.39	0.57
1:A:469:LEU:O	1:A:472:PHE:HB2	2.04	0.57
1:A:561:PHE:HE1	1:A:678:VAL:HB	1.69	0.57
1:A:51:PRO:CG	1:A:673:SER:HB2	2.34	0.57
1:A:102:ASP:OD2	1:A:577:TYR:OH	2.22	0.57
1:A:641:LYS:HG2	1:A:642:GLU:HG3	1.85	0.57
1:A:805:ILE:HD11	1:A:886:PRO:HG2	1.87	0.57
1:A:253:ARG:HG3	4:A:1361:HOH:O	2.05	0.57
1:A:424:LEU:HB2	1:A:425:PRO:HD3	1.86	0.57
1:A:754:ASN:ND2	4:A:1349:HOH:O	2.36	0.57
1:A:345:VAL:O	1:A:347:PRO:HD3	2.05	0.57
1:A:393:PRO:HG2	1:A:428:PRO:HA	1.86	0.57
1:A:553:PHE:N	4:A:1336:HOH:O	2.27	0.57
1:A:423:VAL:HG13	1:A:424:LEU:HD13	1.85	0.56
1:A:1024:ILE:O	1:A:1028:THR:N	2.36	0.56
1:A:24:TRP:CD1	1:A:29:VAL:HG21	2.40	0.56
1:A:465:GLU:O	1:A:468:TYR:HB2	2.05	0.56
1:A:240:TYR:HA	1:A:247:PRO:HA	1.87	0.56
1:A:770:TRP:HE1	1:A:870:ILE:HD12	1.70	0.56
1:A:193:LYS:HG2	1:A:201:TRP:CZ2	2.40	0.56
1:A:717:MET:HA	1:A:723:ASN:O	2.06	0.56
1:A:160:ILE:HA	1:A:163:SER:HB2	1.88	0.56
1:A:825:PHE:CD1	1:A:859:LEU:HD13	2.41	0.56
1:A:1046:ASP:OD1	1:A:1049:ARG:NH1	2.39	0.56
1:A:254:GLN:HB2	1:A:515:MET:HB2	1.86	0.56
1:A:304:ASN:N	1:A:391:SER:OG	2.35	0.56
1:A:415:LYS:HG2	1:A:416:TYR:CD2	2.41	0.56
1:A:367:THR:C	1:A:369:TYR:H	2.13	0.56
1:A:508:MET:HB3	1:A:523:VAL:CG1	2.34	0.56
1:A:601:MET:HB2	1:A:666:TYR:OH	2.06	0.56
1:A:74:VAL:HB	1:A:84:CYS:SG	2.46	0.55
1:A:97:ILE:HD12	1:A:97:ILE:H	1.71	0.55
1:A:1041:ALA:HA	1:A:1044:ALA:HB2	1.87	0.55
1:A:299:MET:HE2	1:A:299:MET:HA	1.88	0.55
1:A:959:PHE:C	1:A:961:ALA:H	2.14	0.55
1:A:174:PHE:HB3	1:A:180:TRP:NE1	2.15	0.55
1:A:418:ILE:HA	1:A:422:MET:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:LYS:HA	1:A:970:LYS:HE3	1.85	0.55
1:A:11:ASP:O	1:A:14:LYS:N	2.40	0.55
1:A:460:LEU:HD22	4:A:1545:HOH:O	2.07	0.55
1:A:1029:ASN:C	1:A:1031:LEU:H	2.13	0.55
1:A:1036:ILE:HD13	4:A:1384:HOH:O	2.06	0.55
1:A:396:SER:HB2	1:A:464:LYS:NZ	2.22	0.55
1:A:607:ALA:O	1:A:611:GLN:HG3	2.06	0.55
1:A:645:PHE:CE1	1:A:652:LYS:HG3	2.41	0.55
1:A:293:THR:OG1	2:A:1202:LEU:N	2.39	0.55
1:A:313:TYR:O	1:A:352:LEU:HD23	2.05	0.55
1:A:581:THR:O	1:A:591:ILE:HG13	2.06	0.55
1:A:214:TYR:OH	1:A:596:ASP:O	2.24	0.55
1:A:332:ARG:O	1:A:335:SER:OG	2.23	0.55
1:A:238:THR:HG21	1:A:247:PRO:HB2	1.89	0.55
1:A:766:ARG:HD3	1:A:829:GLN:HG3	1.88	0.55
1:A:191:ASP:OD2	1:A:728:THR:HB	2.07	0.55
1:A:45:LYS:NZ	1:A:669:ASP:OD2	2.38	0.54
1:A:419:ARG:HB3	4:A:1437:HOH:O	2.07	0.54
1:A:719:LYS:HD3	1:A:719:LYS:N	2.22	0.54
1:A:162:LYS:NZ	1:A:168:ASP:HB3	2.23	0.54
1:A:404:ARG:HB3	1:A:408:LYS:NZ	2.22	0.54
1:A:634:VAL:HG12	1:A:646:PRO:CG	2.38	0.54
1:A:238:THR:HG22	1:A:239:ILE:O	2.07	0.54
1:A:51:PRO:HG3	1:A:671:ARG:HE	1.73	0.54
1:A:58:ARG:CZ	1:A:187:LEU:HD13	2.38	0.54
1:A:798:ALA:HB2	1:A:847:LEU:CD1	2.37	0.54
1:A:70:CYS:O	1:A:74:VAL:HG13	2.07	0.54
1:A:89:GLY:N	1:A:604:TYR:OH	2.41	0.54
1:A:102:ASP:HA	1:A:105:LYS:HG3	1.90	0.53
1:A:231:ILE:HG23	1:A:532:LEU:HD23	1.90	0.53
1:A:417:GLY:O	1:A:422:MET:HE2	2.08	0.53
1:A:416:TYR:H	1:A:418:ILE:HG13	1.72	0.53
1:A:825:PHE:CE1	1:A:859:LEU:HD13	2.43	0.53
1:A:211:ASN:HA	1:A:616:HIS:O	2.08	0.53
1:A:222:PHE:CE2	1:A:591:ILE:HD13	2.43	0.53
1:A:433:GLU:HB2	1:A:478:LEU:HD11	1.89	0.53
1:A:531:TYR:HB2	1:A:571:HIS:O	2.07	0.53
1:A:869:HIS:O	1:A:873:LEU:N	2.39	0.53
1:A:894:VAL:O	4:A:1321:HOH:O	2.19	0.53
1:A:195:MET:HE3	1:A:197:LEU:HD21	1.90	0.53
1:A:606:VAL:HB	1:A:610:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:LYS:CE	1:A:943:ASN:HB2	2.39	0.53
1:A:405:ASP:CB	1:A:454:GLN:HE21	2.21	0.53
1:A:457:ARG:HD3	1:A:457:ARG:N	2.24	0.53
1:A:1049:ARG:NH2	4:A:1355:HOH:O	2.40	0.53
1:A:638:VAL:C	1:A:659:LYS:HZ3	2.09	0.53
1:A:254:GLN:N	1:A:515:MET:O	2.42	0.52
1:A:848:VAL:HG12	1:A:849:PHE:HD1	1.74	0.52
1:A:905:VAL:HA	1:A:908:ASP:CB	2.39	0.52
1:A:218:VAL:CG1	1:A:581:THR:HG21	2.39	0.52
1:A:405:ASP:OD2	1:A:454:GLN:HB2	2.10	0.52
1:A:314:ILE:HD13	1:A:351:GLU:HA	1.90	0.52
1:A:391:SER:O	1:A:393:PRO:HD3	2.09	0.52
1:A:409:LYS:HG3	1:A:411:ALA:C	2.34	0.52
1:A:746:ALA:O	1:A:753:ALA:HB1	2.08	0.52
1:A:905:VAL:HA	1:A:908:ASP:HB3	1.91	0.52
1:A:1032:GLU:HG3	4:A:1317:HOH:O	2.09	0.52
1:A:608:HIS:CE1	1:A:609:LEU:HG	2.45	0.52
1:A:868:GLU:OE1	1:A:872:THR:HG23	2.10	0.52
1:A:289:LEU:HD12	1:A:362:LEU:HD21	1.91	0.52
1:A:409:LYS:H	1:A:409:LYS:NZ	2.02	0.52
1:A:458:GLU:O	1:A:461:ALA:HB3	2.10	0.52
1:A:676:ASP:OD1	1:A:676:ASP:N	2.43	0.52
1:A:1041:ALA:HA	1:A:1044:ALA:CB	2.39	0.52
1:A:1041:ALA:HB1	1:A:1049:ARG:HB2	1.91	0.52
1:A:335:SER:HB2	1:A:344:GLY:C	2.34	0.52
1:A:349:VAL:O	1:A:350:LYS:HG3	2.09	0.52
1:A:745:ASP:C	1:A:747:GLY:H	2.17	0.52
1:A:895:LEU:O	1:A:898:SER:OG	2.21	0.52
1:A:286:ASN:HB3	1:A:288:PHE:CE1	2.45	0.52
1:A:989:VAL:O	1:A:993:VAL:HB	2.10	0.52
1:A:418:ILE:HG23	1:A:422:MET:HG2	1.92	0.51
1:A:419:ARG:NH1	4:A:1333:HOH:O	2.26	0.51
1:A:359:GLY:H	1:A:374:VAL:HG13	1.75	0.51
1:A:397:PRO:CB	1:A:463:ALA:HB1	2.39	0.51
1:A:531:TYR:HA	1:A:573:CYS:SG	2.51	0.51
1:A:212:PRO:HG2	1:A:213:TYR:CD1	2.45	0.51
1:A:487:VAL:N	4:A:1367:HOH:O	2.43	0.51
1:A:639:PHE:C	1:A:659:LYS:HZ1	2.17	0.51
1:A:217:PHE:CE2	1:A:600:TYR:HA	2.37	0.51
1:A:240:TYR:HB3	1:A:524:VAL:CG1	2.41	0.51
1:A:609:LEU:HB2	1:A:658:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PHE:HB3	1:A:611:GLN:NE2	1.99	0.51
1:A:21:GLN:NE2	1:A:194:ARG:O	2.41	0.51
1:A:201:TRP:HA	1:A:201:TRP:CE3	2.46	0.51
1:A:767:LEU:HD22	1:A:866:LEU:CD1	2.41	0.51
1:A:565:LEU:C	1:A:567:TRP:H	2.18	0.51
1:A:731:ILE:HG23	1:A:736:ALA:HB2	1.92	0.51
1:A:876:LYS:HD2	1:A:877:PRO:HD3	1.93	0.51
1:A:945:PRO:HG2	1:A:948:GLN:HG3	1.92	0.51
1:A:947:TRP:CZ3	1:A:988:LYS:HB3	2.46	0.51
1:A:977:GLY:HA2	1:A:986:MET:HE2	1.93	0.51
1:A:316:PHE:HB2	1:A:347:PRO:O	2.11	0.50
1:A:795:ARG:NH1	4:A:1372:HOH:O	2.44	0.50
1:A:306:TRP:CH2	1:A:402:ALA:HB1	2.46	0.50
1:A:825:PHE:HE1	1:A:859:LEU:HD22	1.76	0.50
1:A:1000:LEU:HD21	1:A:1007:ILE:H	1.76	0.50
1:A:392:VAL:N	1:A:399:ASP:OD2	2.44	0.50
1:A:449:LEU:HD11	1:A:466:LYS:NZ	2.26	0.50
1:A:328:GLN:N	4:A:1360:HOH:O	2.42	0.50
1:A:400:ILE:HD12	1:A:443:VAL:HG13	1.94	0.50
1:A:437:PHE:HB2	4:A:1488:HOH:O	2.11	0.50
1:A:634:VAL:HG12	1:A:646:PRO:HG2	1.94	0.50
1:A:775:LYS:O	1:A:778:VAL:HG12	2.11	0.50
1:A:956:ARG:HG2	1:A:1008:LEU:HD23	1.92	0.50
1:A:415:LYS:N	1:A:418:ILE:HG13	2.27	0.50
1:A:463:ALA:O	1:A:466:LYS:HB2	2.12	0.50
1:A:1040:PHE:HB3	1:A:1042:SER:HB2	1.93	0.50
1:A:314:ILE:O	1:A:325:ILE:HA	2.12	0.50
1:A:949:HIS:CD2	1:A:949:HIS:N	2.77	0.50
1:A:69:LYS:HE3	1:A:705:ARG:NH2	2.27	0.50
1:A:372:ILE:HA	1:A:426:PHE:CZ	2.47	0.50
1:A:379:THR:HG23	4:A:1390:HOH:O	2.11	0.50
1:A:791:THR:OG1	1:A:792:PHE:N	2.45	0.50
1:A:1001:GLU:O	1:A:1001:GLU:HG3	2.12	0.50
1:A:496:LYS:HA	1:A:499:ILE:HG13	1.94	0.49
1:A:52:TYR:HD2	1:A:89:GLY:HA3	1.78	0.49
1:A:156:TYR:N	4:A:1380:HOH:O	2.46	0.49
1:A:168:ASP:OD1	1:A:168:ASP:N	2.45	0.49
1:A:211:ASN:ND2	1:A:617:GLY:HA3	2.27	0.49
1:A:287:ILE:HG23	1:A:323:ILE:CB	2.41	0.49
1:A:373:TYR:CG	1:A:422:MET:SD	3.05	0.49
1:A:939:TYR:HD1	1:A:1039:LYS:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLU:HG2	1:A:275:TYR:CE1	2.47	0.49
1:A:412:LEU:HD23	1:A:415:LYS:HD2	1.93	0.49
1:A:237:TYR:HA	1:A:524:VAL:O	2.13	0.49
1:A:415:LYS:HE2	1:A:416:TYR:CE1	2.47	0.49
1:A:685:TYR:OH	1:A:701:PRO:HB3	2.12	0.49
1:A:791:THR:O	1:A:794:ASP:HB2	2.12	0.49
1:A:807:LYS:HA	1:A:810:GLN:OE1	2.12	0.49
1:A:989:VAL:O	1:A:993:VAL:N	2.45	0.49
1:A:246:GLN:OE1	1:A:577:TYR:N	2.27	0.49
1:A:397:PRO:O	1:A:398:ASP:C	2.55	0.49
1:A:530:TRP:HD1	1:A:589:TRP:NE1	2.11	0.49
1:A:731:ILE:HD13	1:A:736:ALA:HB2	1.94	0.49
1:A:424:LEU:HD22	1:A:424:LEU:H	1.77	0.49
1:A:201:TRP:HA	1:A:201:TRP:HE3	1.77	0.49
1:A:688:ASN:O	1:A:691:ALA:N	2.45	0.49
1:A:55:MET:O	1:A:184:PHE:HD2	1.95	0.49
1:A:837:GLU:OE1	1:A:837:GLU:HA	2.13	0.49
1:A:67:LEU:HD12	1:A:68:SER:N	2.28	0.49
1:A:272:LEU:HD11	1:A:363:SER:CB	2.42	0.49
1:A:313:TYR:N	1:A:352:LEU:O	2.33	0.49
1:A:631:THR:O	1:A:634:VAL:HG22	2.13	0.49
1:A:645:PHE:HE1	1:A:655:LEU:HD13	1.77	0.49
1:A:848:VAL:HG12	1:A:849:PHE:CD1	2.48	0.49
1:A:207:THR:HA	1:A:214:TYR:CD2	2.48	0.49
1:A:608:HIS:O	1:A:622:PRO:HG2	2.12	0.49
1:A:158:TRP:CH2	1:A:171:ILE:HB	2.47	0.48
1:A:72:PHE:CB	1:A:817:PHE:CE2	2.93	0.48
1:A:469:LEU:O	1:A:472:PHE:N	2.38	0.48
1:A:699:LYS:N	4:A:1339:HOH:O	2.46	0.48
1:A:85:LEU:HD22	1:A:665:TRP:CE2	2.48	0.48
1:A:249:MET:H	1:A:575:ARG:NH2	2.11	0.48
1:A:396:SER:HA	1:A:464:LYS:HE2	1.94	0.48
1:A:568:LEU:HD21	1:A:684:TYR:CE1	2.47	0.48
1:A:98:LYS:O	1:A:102:ASP:HB2	2.14	0.48
1:A:207:THR:HG22	1:A:214:TYR:CZ	2.48	0.48
1:A:868:GLU:OE2	1:A:880:ILE:HG22	2.13	0.48
1:A:939:TYR:CD1	1:A:1039:LYS:HB2	2.48	0.48
1:A:988:LYS:HE2	1:A:1051:ASP:OD1	2.13	0.48
1:A:158:TRP:HZ3	1:A:172:VAL:HG13	1.79	0.48
1:A:325:ILE:N	1:A:325:ILE:HD12	2.29	0.48
1:A:666:TYR:CD2	1:A:667:PRO:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ASP:OD2	1:A:818:LYS:N	2.45	0.48
1:A:55:MET:HE3	1:A:90:LEU:HD21	1.95	0.48
1:A:227:GLU:OE1	1:A:632:LYS:HE3	2.12	0.48
1:A:228:ARG:HG2	4:A:1644:HOH:O	2.14	0.48
1:A:434:ILE:HG23	1:A:474:GLU:HB3	1.96	0.48
1:A:938:ILE:HG23	1:A:1059:ASN:HB3	1.95	0.48
1:A:240:TYR:CD2	1:A:524:VAL:HG21	2.49	0.48
1:A:262:GLN:HB2	1:A:511:GLU:HG3	1.94	0.48
1:A:855:GLN:OE1	4:A:1323:HOH:O	2.20	0.48
1:A:295:ARG:HB3	1:A:298:THR:HG23	1.96	0.48
1:A:158:TRP:CZ3	1:A:172:VAL:HG13	2.48	0.48
1:A:806:ILE:O	1:A:807:LYS:C	2.57	0.48
1:A:872:THR:HG22	4:A:1328:HOH:O	2.14	0.48
1:A:220:TRP:HA	1:A:223:LEU:HD12	1.95	0.47
1:A:282:LEU:HD12	1:A:282:LEU:H	1.79	0.47
1:A:295:ARG:HH22	1:A:464:LYS:HD2	1.78	0.47
1:A:603:PHE:HZ	1:A:611:GLN:OE1	1.84	0.47
1:A:1012:LEU:O	1:A:1014:PHE:N	2.47	0.47
1:A:434:ILE:HG12	1:A:475:GLY:HA2	1.94	0.47
1:A:754:ASN:OD1	1:A:755:PHE:N	2.47	0.47
1:A:819:GLU:O	1:A:823:THR:HG23	2.14	0.47
1:A:93:THR:HG23	1:A:580:GLY:HA2	1.96	0.47
1:A:299:MET:HE2	1:A:302:GLN:HG3	1.96	0.47
1:A:543:THR:HG21	1:A:687:TYR:HA	1.96	0.47
1:A:693:TRP:CD1	1:A:696:GLN:HG3	2.38	0.47
1:A:835:TYR:O	1:A:835:TYR:CG	2.68	0.47
1:A:1048:ILE:HG23	1:A:1058:LEU:HB2	1.94	0.47
1:A:107:GLU:O	1:A:111:TYR:HD2	1.97	0.47
1:A:236:ARG:HH11	1:A:236:ARG:HA	1.79	0.47
1:A:299:MET:HB3	1:A:302:GLN:OE1	2.14	0.47
1:A:218:VAL:HG11	1:A:581:THR:HG21	1.95	0.47
1:A:221:GLN:HE22	1:A:599:ILE:HG23	1.79	0.47
1:A:302:GLN:NE2	1:A:364:ALA:HB1	2.30	0.47
1:A:314:ILE:HG23	1:A:348:VAL:HG23	1.96	0.47
1:A:101:ALA:N	4:A:1311:HOH:O	2.20	0.47
1:A:235:LYS:HE2	1:A:527:CYS:HA	1.97	0.47
1:A:600:TYR:CD1	1:A:600:TYR:C	2.93	0.47
1:A:909:LEU:HA	4:A:1307:HOH:O	2.14	0.47
1:A:976:LEU:O	1:A:982:LEU:HD23	2.14	0.47
1:A:24:TRP:HZ3	1:A:865:HIS:CD2	2.33	0.47
1:A:61:LEU:HA	1:A:61:LEU:HD23	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:THR:HG21	4:A:1545:HOH:O	2.14	0.47
1:A:78:ARG:HD3	1:A:881:MET:CE	2.45	0.47
1:A:352:LEU:HA	4:A:1365:HOH:O	2.14	0.47
1:A:161:MET:HB3	1:A:171:ILE:CG2	2.46	0.46
1:A:391:SER:OG	1:A:391:SER:O	2.32	0.46
1:A:400:ILE:HD12	1:A:443:VAL:HG22	1.97	0.46
1:A:550:LEU:HD12	1:A:701:PRO:O	2.14	0.46
1:A:269:LEU:HD12	1:A:289:LEU:O	2.15	0.46
1:A:468:TYR:HB3	1:A:469:LEU:H	1.63	0.46
1:A:739:MET:HE3	1:A:739:MET:HB3	1.64	0.46
1:A:323:ILE:HD12	1:A:323:ILE:HG23	1.68	0.46
1:A:978:SER:O	1:A:978:SER:OG	2.32	0.46
1:A:818:LYS:O	1:A:821:LEU:HB3	2.15	0.46
1:A:716:LYS:HD2	1:A:716:LYS:HA	1.73	0.46
1:A:636:ASP:O	1:A:640:PHE:HB2	2.15	0.46
1:A:641:LYS:HA	1:A:659:LYS:CE	2.46	0.46
1:A:821:LEU:HD21	1:A:826:PHE:HE1	1.81	0.46
1:A:58:ARG:HA	4:A:1536:HOH:O	2.15	0.46
1:A:409:LYS:HE3	1:A:409:LYS:HB3	1.82	0.46
1:A:594:LEU:HD23	1:A:594:LEU:HA	1.51	0.46
1:A:47:PHE:O	1:A:669:ASP:HB2	2.16	0.46
1:A:231:ILE:HG23	1:A:532:LEU:CD2	2.45	0.46
1:A:267:LEU:HD13	1:A:365:PRO:HG2	1.98	0.46
1:A:584:PRO:HB2	1:A:585:TRP:HE3	1.80	0.46
1:A:86:PHE:HB3	1:A:198:LYS:O	2.16	0.46
1:A:192:LEU:O	1:A:196:GLY:N	2.49	0.46
1:A:299:MET:HE1	1:A:390:THR:CB	2.45	0.46
1:A:594:LEU:HD21	1:A:681:HIS:HB2	1.98	0.46
1:A:601:MET:HE2	1:A:671:ARG:CZ	2.45	0.46
1:A:194:ARG:NE	4:A:1343:HOH:O	2.37	0.46
1:A:786:SER:OG	1:A:787:GLY:N	2.49	0.46
1:A:52:TYR:HD1	1:A:52:TYR:O	1.99	0.45
1:A:58:ARG:NE	1:A:187:LEU:HB3	2.30	0.45
1:A:235:LYS:HG3	1:A:527:CYS:HA	1.97	0.45
1:A:473:TYR:HD2	1:A:488:GLN:OE1	1.99	0.45
1:A:543:THR:HG22	1:A:690:VAL:HG21	1.98	0.45
1:A:219:ARG:NH1	1:A:584:PRO:HA	2.31	0.45
1:A:415:LYS:HE2	1:A:416:TYR:CZ	2.51	0.45
1:A:583:LEU:HD12	1:A:589:TRP:CB	2.46	0.45
1:A:594:LEU:HD11	1:A:680:ASN:OD1	2.16	0.45
1:A:781:TRP:C	1:A:783:SER:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ILE:HG22	1:A:1048:ILE:O	2.17	0.45
1:A:76:TYR:OH	1:A:813:GLU:HG3	2.16	0.45
1:A:239:ILE:HD13	1:A:249:MET:HE3	1.98	0.45
1:A:673:SER:OG	1:A:674:GLY:N	2.49	0.45
1:A:717:MET:HG2	1:A:724:PHE:CD2	2.52	0.45
1:A:745:ASP:HB3	1:A:759:MET:HE1	1.99	0.45
1:A:34:ALA:O	1:A:38:GLU:HB2	2.16	0.45
1:A:82:LYS:HD3	4:A:1387:HOH:O	2.17	0.45
1:A:90:LEU:HA	1:A:90:LEU:HD23	1.65	0.45
1:A:540:LYS:HG3	1:A:687:TYR:OH	2.15	0.45
1:A:686:LEU:HD23	1:A:686:LEU:HA	1.67	0.45
1:A:731:ILE:HG12	1:A:739:MET:HE2	1.97	0.45
1:A:885:TRP:CG	1:A:886:PRO:HD2	2.51	0.45
1:A:72:PHE:HB2	1:A:817:PHE:HE2	1.79	0.45
1:A:749:THR:OG1	1:A:750:VAL:N	2.50	0.45
1:A:161:MET:HB3	1:A:171:ILE:HG23	1.99	0.45
1:A:215:ASP:O	1:A:218:VAL:HG12	2.15	0.45
1:A:645:PHE:HE1	1:A:655:LEU:CD1	2.29	0.45
1:A:872:THR:HA	4:A:1328:HOH:O	2.15	0.45
1:A:55:MET:CG	1:A:90:LEU:HD22	2.44	0.45
1:A:1040:PHE:HD1	1:A:1040:PHE:O	2.00	0.45
1:A:93:THR:HG22	1:A:94:GLY:N	2.28	0.45
1:A:194:ARG:CZ	1:A:731:ILE:HG22	2.46	0.45
1:A:329:LYS:HA	1:A:329:LYS:HD3	1.68	0.45
1:A:55:MET:HE1	1:A:188:ALA:HB2	1.99	0.45
1:A:499:ILE:HA	1:A:504:ALA:O	2.16	0.45
1:A:550:LEU:HD13	1:A:686:LEU:HD21	1.99	0.45
1:A:802:ASN:O	1:A:805:ILE:HG22	2.16	0.45
1:A:104:LEU:HD11	1:A:158:TRP:HE3	1.82	0.45
1:A:670:LEU:HA	1:A:703:ALA:O	2.17	0.45
1:A:870:ILE:HA	1:A:873:LEU:HB2	1.99	0.45
1:A:61:LEU:HA	1:A:64:THR:CG2	2.47	0.44
1:A:397:PRO:HD2	1:A:464:LYS:HE3	1.98	0.44
1:A:513:GLN:OE1	1:A:515:MET:HE2	2.16	0.44
1:A:821:LEU:CD2	1:A:826:PHE:HE1	2.29	0.44
1:A:829:GLN:HG2	4:A:1323:HOH:O	2.16	0.44
1:A:955:LEU:HD13	1:A:955:LEU:HA	1.78	0.44
1:A:10:VAL:HG11	1:A:733:LYS:O	2.17	0.44
1:A:298:THR:HG22	1:A:432:ILE:HD13	2.00	0.44
1:A:707:ASN:OD1	1:A:707:ASN:N	2.50	0.44
1:A:956:ARG:HH12	1:A:1010:LEU:HD22	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HE2	1:A:577:TYR:OH	2.17	0.44
1:A:358:LEU:HA	1:A:374:VAL:HG13	1.99	0.44
1:A:969:ASN:CA	1:A:972:ILE:HG13	2.46	0.44
1:A:358:LEU:H	1:A:358:LEU:HG	1.15	0.44
1:A:369:TYR:HB3	1:A:372:ILE:HG23	1.99	0.44
1:A:380:ILE:O	1:A:382:GLU:HG2	2.18	0.44
1:A:434:ILE:CG2	1:A:474:GLU:HB3	2.48	0.44
1:A:532:LEU:HG	1:A:573:CYS:SG	2.57	0.44
1:A:755:PHE:CD1	1:A:755:PHE:C	2.95	0.44
1:A:195:MET:CE	1:A:197:LEU:HD21	2.47	0.44
1:A:220:TRP:O	1:A:221:GLN:C	2.60	0.44
1:A:316:PHE:HA	1:A:349:VAL:HG13	2.00	0.44
1:A:536:GLU:HB2	1:A:539:TRP:HB3	2.00	0.44
1:A:306:TRP:HA	1:A:375:LEU:O	2.17	0.44
1:A:52:TYR:CZ	1:A:207:THR:HG21	2.53	0.44
1:A:60:HIS:O	1:A:64:THR:HG23	2.17	0.44
1:A:241:SER:O	1:A:242:PRO:C	2.61	0.44
1:A:354:GLY:O	1:A:358:LEU:HG	2.17	0.44
1:A:431:VAL:HG23	1:A:432:ILE:HD12	2.00	0.44
1:A:1016:GLU:O	1:A:1017:LYS:C	2.61	0.44
1:A:958:HIS:ND1	1:A:958:HIS:C	2.73	0.44
1:A:200:ASP:OD2	1:A:203:ARG:NE	2.50	0.44
1:A:275:TYR:HB3	1:A:279:LEU:HD12	2.00	0.44
1:A:298:THR:HG22	1:A:432:ILE:CD1	2.48	0.44
1:A:777:MET:HE3	1:A:777:MET:HB2	1.76	0.44
1:A:843:MET:HE2	1:A:843:MET:HB3	1.79	0.44
1:A:161:MET:HE3	1:A:180:TRP:CZ2	2.53	0.43
1:A:677:LEU:O	1:A:682:LEU:HD12	2.18	0.43
1:A:48:VAL:HG23	1:A:86:PHE:HA	2.00	0.43
1:A:477:MET:HG2	1:A:487:VAL:HG22	2.00	0.43
1:A:495:GLN:NE2	1:A:506:ILE:HD11	2.33	0.43
1:A:745:ASP:C	1:A:747:GLY:N	2.76	0.43
1:A:172:VAL:C	1:A:174:PHE:H	2.25	0.43
1:A:532:LEU:O	1:A:570:GLU:HB3	2.19	0.43
1:A:665:TRP:HA	1:A:665:TRP:CE3	2.53	0.43
1:A:692:MET:C	1:A:694:PRO:HD3	2.42	0.43
1:A:1029:ASN:O	1:A:1031:LEU:N	2.52	0.43
1:A:183:TYR:C	1:A:186:PRO:HD2	2.43	0.43
1:A:415:LYS:HG2	1:A:416:TYR:CZ	2.54	0.43
1:A:770:TRP:O	1:A:771:VAL:C	2.62	0.43
1:A:938:ILE:O	1:A:1038:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:C	1:A:174:PHE:N	2.77	0.43
1:A:240:TYR:O	1:A:242:PRO:HD3	2.19	0.43
1:A:266:LEU:HD21	1:A:290:VAL:CB	2.46	0.43
1:A:291:ALA:HB2	1:A:388:VAL:HB	2.00	0.43
1:A:672:VAL:HG23	1:A:705:ARG:O	2.18	0.43
1:A:729:GLN:O	1:A:730:ALA:C	2.60	0.43
1:A:60:HIS:CE1	1:A:63:HIS:CE1	3.06	0.43
1:A:806:ILE:O	1:A:809:ASP:N	2.52	0.43
1:A:847:LEU:HD23	1:A:847:LEU:HA	1.82	0.43
1:A:69:LYS:CE	1:A:705:ARG:HH21	2.29	0.43
1:A:85:LEU:HD22	1:A:665:TRP:CD2	2.54	0.43
1:A:221:GLN:HB2	1:A:599:ILE:CD1	2.48	0.43
1:A:264:TYR:CB	1:A:292:ALA:HB1	2.48	0.43
1:A:378:LEU:N	4:A:1390:HOH:O	2.52	0.43
1:A:735:SER:O	1:A:736:ALA:C	2.62	0.43
1:A:231:ILE:O	1:A:232:LYS:HG3	2.19	0.43
1:A:253:ARG:NH2	1:A:259:VAL:HB	2.34	0.43
1:A:814:LYS:O	1:A:816:MET:HG3	2.19	0.43
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.59	0.43
1:A:811:ASN:HB2	1:A:820:ALA:CB	2.40	0.43
1:A:92:CYS:HB3	1:A:181:LEU:HD21	2.00	0.42
1:A:211:ASN:HD22	1:A:617:GLY:HA3	1.83	0.42
1:A:956:ARG:HG3	1:A:1008:LEU:CD2	2.49	0.42
1:A:958:HIS:CE1	1:A:967:PRO:HD3	2.54	0.42
1:A:194:ARG:NH2	4:A:1343:HOH:O	2.30	0.42
1:A:449:LEU:HD11	1:A:466:LYS:CE	2.49	0.42
1:A:896:ILE:O	1:A:899:SER:N	2.52	0.42
1:A:208:THR:HG22	1:A:580:GLY:HA2	2.02	0.42
1:A:526:LEU:C	1:A:528:ASP:H	2.26	0.42
1:A:635:TRP:CD1	4:A:1377:HOH:O	2.72	0.42
1:A:735:SER:O	1:A:737:ASP:N	2.53	0.42
1:A:405:ASP:CG	1:A:454:GLN:HE21	2.28	0.42
1:A:498:MET:HG2	1:A:504:ALA:HB2	2.02	0.42
1:A:1014:PHE:N	1:A:1014:PHE:CD1	2.88	0.42
1:A:262:GLN:HB2	1:A:511:GLU:CG	2.49	0.42
1:A:352:LEU:CD1	1:A:357:ILE:HD11	2.36	0.42
1:A:414:ALA:C	1:A:418:ILE:HG13	2.44	0.42
1:A:780:ASN:HB3	1:A:783:SER:HB3	2.02	0.42
1:A:832:LYS:HE2	1:A:833:ASP:OD1	2.19	0.42
1:A:945:PRO:HB2	1:A:947:TRP:CD1	2.55	0.42
1:A:98:LYS:HE2	1:A:577:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLN:HE22	1:A:161:MET:HE1	1.85	0.42
1:A:268:LYS:HD2	1:A:288:PHE:CG	2.55	0.42
1:A:358:LEU:HD13	1:A:416:TYR:CD2	2.55	0.42
1:A:196:GLY:C	1:A:197:LEU:HD23	2.44	0.42
1:A:220:TRP:HB3	4:A:1377:HOH:O	2.20	0.42
1:A:268:LYS:HD2	1:A:288:PHE:CD2	2.54	0.42
1:A:306:TRP:HD1	1:A:390:THR:O	2.01	0.42
1:A:1015:ASP:O	1:A:1019:VAL:HG13	2.19	0.42
1:A:1017:LYS:NZ	1:A:1021:MET:HG3	2.34	0.42
1:A:45:LYS:HE2	1:A:667:PRO:HD2	2.00	0.42
1:A:248:CYS:HA	1:A:575:ARG:NH2	2.35	0.42
1:A:314:ILE:HD13	1:A:314:ILE:HA	1.70	0.42
1:A:408:LYS:HZ3	1:A:408:LYS:HG3	1.62	0.42
1:A:779:ALA:O	1:A:781:TRP:N	2.45	0.42
1:A:866:LEU:C	1:A:866:LEU:HD23	2.45	0.42
1:A:102:ASP:O	1:A:105:LYS:HG3	2.19	0.42
1:A:185:PRO:HG2	1:A:206:ILE:HD11	2.02	0.42
1:A:266:LEU:HD23	1:A:267:LEU:N	2.34	0.42
1:A:464:LYS:HE3	4:A:1389:HOH:O	2.19	0.42
1:A:593:SER:O	1:A:595:SER:N	2.52	0.42
1:A:844:HIS:CE1	1:A:846:GLU:H	2.38	0.42
1:A:938:ILE:HD12	1:A:1059:ASN:CB	2.48	0.42
1:A:11:ASP:O	1:A:12:PHE:C	2.63	0.42
1:A:811:ASN:ND2	4:A:1341:HOH:O	2.28	0.42
1:A:934:SER:O	1:A:1033:LEU:HB3	2.19	0.42
1:A:52:TYR:CE1	1:A:91:HIS:CD2	3.07	0.41
1:A:215:ASP:HA	1:A:218:VAL:HG12	2.02	0.41
1:A:316:PHE:CE1	1:A:324:PHE:HB3	2.55	0.41
1:A:377:MET:HG2	1:A:380:ILE:HG13	2.02	0.41
1:A:404:ARG:C	1:A:408:LYS:HZ3	2.28	0.41
1:A:413:ARG:O	1:A:413:ARG:HG2	2.19	0.41
1:A:871:TRP:CE2	1:A:876:LYS:HB3	2.55	0.41
1:A:981:GLU:H	1:A:981:GLU:HG3	1.52	0.41
1:A:111:TYR:CE1	1:A:117:PHE:HZ	2.38	0.41
1:A:249:MET:O	1:A:253:ARG:CZ	2.68	0.41
1:A:267:LEU:HD21	1:A:498:MET:SD	2.59	0.41
1:A:290:VAL:HG22	1:A:325:ILE:O	2.20	0.41
1:A:394:SER:OG	1:A:429:VAL:N	2.52	0.41
1:A:537:GLU:N	4:A:1362:HOH:O	2.42	0.41
1:A:594:LEU:CD2	1:A:681:HIS:HB2	2.50	0.41
1:A:50:PHE:HD2	1:A:88:PHE:CE1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HH11	1:A:219:ARG:HG2	1.85	0.41
1:A:223:LEU:HD21	1:A:584:PRO:HB3	2.02	0.41
1:A:246:GLN:HB2	1:A:575:ARG:HD2	2.01	0.41
1:A:670:LEU:HD11	1:A:815:MET:HE1	2.02	0.41
1:A:770:TRP:CH2	1:A:855:GLN:HG2	2.55	0.41
1:A:949:HIS:H	1:A:949:HIS:HD2	1.62	0.41
1:A:829:GLN:HE21	1:A:829:GLN:HA	1.85	0.41
1:A:306:TRP:HE1	1:A:391:SER:HA	1.85	0.41
1:A:510:PRO:HD3	1:A:523:VAL:HG23	2.01	0.41
1:A:514:VAL:HB	1:A:521:GLU:HG3	2.03	0.41
1:A:719:LYS:HD3	1:A:719:LYS:H	1.84	0.41
1:A:843:MET:O	4:A:1326:HOH:O	2.21	0.41
1:A:939:TYR:HA	1:A:1039:LYS:O	2.20	0.41
1:A:41:THR:HG23	4:A:1609:HOH:O	2.21	0.41
1:A:92:CYS:SG	1:A:206:ILE:HG23	2.61	0.41
1:A:513:GLN:HG2	1:A:514:VAL:N	2.35	0.41
1:A:570:GLU:H	1:A:570:GLU:CD	2.28	0.41
1:A:705:ARG:NH2	1:A:748:ASP:O	2.54	0.41
1:A:960:GLU:OE1	1:A:960:GLU:HA	2.20	0.41
1:A:238:THR:CG2	1:A:247:PRO:HB2	2.49	0.41
1:A:261:PRO:HB3	1:A:523:VAL:HG13	2.02	0.41
1:A:325:ILE:HD12	1:A:325:ILE:H	1.85	0.41
1:A:1014:PHE:N	1:A:1014:PHE:HD1	2.19	0.41
1:A:93:THR:HG23	1:A:580:GLY:CA	2.50	0.41
1:A:230:LYS:HZ2	1:A:539:TRP:CD1	2.39	0.41
1:A:836:ARG:HA	1:A:843:MET:HE3	2.03	0.41
1:A:1006:ARG:NH2	4:A:1375:HOH:O	2.45	0.41
1:A:14:LYS:HE3	1:A:194:ARG:NH2	2.35	0.41
1:A:22:GLN:HA	1:A:22:GLN:OE1	2.20	0.41
1:A:52:TYR:CE1	1:A:91:HIS:CG	3.08	0.41
1:A:103:LYS:HG2	1:A:157:GLN:HG2	2.02	0.41
1:A:295:ARG:HB3	1:A:298:THR:CG2	2.51	0.41
1:A:416:TYR:H	1:A:418:ILE:CG1	2.33	0.41
1:A:677:LEU:C	1:A:682:LEU:HD12	2.46	0.41
1:A:784:LEU:CD1	1:A:845:ARG:HB3	2.47	0.41
1:A:858:LEU:HD23	1:A:858:LEU:HA	1.73	0.41
1:A:881:MET:HE2	1:A:881:MET:HA	2.02	0.41
1:A:942:LYS:HE3	1:A:942:LYS:HB3	1.86	0.41
1:A:982:LEU:HD11	1:A:989:VAL:CG2	2.48	0.41
1:A:51:PRO:HA	1:A:671:ARG:NH2	2.36	0.41
1:A:304:ASN:H	1:A:391:SER:HG	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:LEU:HD11	1:A:1033:LEU:HD21	2.03	0.41
1:A:914:LYS:HB3	1:A:914:LYS:HE3	1.93	0.41
1:A:213:TYR:CD2	1:A:610:LEU:O	2.74	0.40
1:A:398:ASP:OD1	1:A:398:ASP:N	2.49	0.40
1:A:455:ASN:HA	1:A:457:ARG:CZ	2.51	0.40
1:A:891:VAL:HG22	1:A:893:GLU:HG2	2.03	0.40
1:A:218:VAL:HG22	1:A:222:PHE:CE2	2.57	0.40
1:A:297:GLU:HG3	1:A:487:VAL:HG13	2.03	0.40
1:A:739:MET:O	1:A:740:ARG:C	2.63	0.40
1:A:868:GLU:OE2	1:A:880:ILE:N	2.35	0.40
1:A:997:LYS:HD3	1:A:997:LYS:HA	1.82	0.40
1:A:52:TYR:HE1	1:A:91:HIS:CD2	2.40	0.40
1:A:459:LYS:O	1:A:462:GLU:HB3	2.22	0.40
1:A:26:THR:HA	4:A:1449:HOH:O	2.22	0.40
1:A:64:THR:HG23	1:A:64:THR:H	1.65	0.40
1:A:184:PHE:HD1	1:A:184:PHE:HA	1.61	0.40
1:A:418:ILE:HG23	1:A:422:MET:CG	2.52	0.40
1:A:513:GLN:CD	1:A:515:MET:HE2	2.46	0.40
1:A:671:ARG:HG2	1:A:672:VAL:N	2.35	0.40
1:A:768:TYR:HA	1:A:771:VAL:HG12	2.02	0.40
1:A:796:VAL:HG12	1:A:895:LEU:HG	2.03	0.40
1:A:990:MET:HB3	1:A:991:PRO:HD3	2.03	0.40
1:A:1000:LEU:HD13	1:A:1004:GLY:O	2.21	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASN:CG	1:A:877:PRO:CG[8_545]	1.09	1.11
1:A:455:ASN:OD1	1:A:877:PRO:CG[8_545]	1.34	0.86
1:A:455:ASN:ND2	1:A:877:PRO:CB[8_545]	1.52	0.68
1:A:455:ASN:ND2	1:A:877:PRO:CG[8_545]	1.65	0.55
1:A:455:ASN:CG	1:A:877:PRO:CB[8_545]	1.89	0.31
1:A:455:ASN:OD1	1:A:877:PRO:CD[8_545]	2.10	0.10

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	996/1188 (84%)	817 (82%)	170 (17%)	9 (1%)	14	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	TYR
1	A	517	ARG
1	A	1013	GLU
1	A	736	ALA
1	A	877	PRO
1	A	960	GLU
1	A	611	GLN
1	A	972	ILE
1	A	186	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/1047 (84%)	722 (82%)	161 (18%)	2	8

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	10	VAL

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Mol	Chain	Res	Type
1	A	20	ILE
1	A	26	THR
1	A	40	GLN
1	A	41	THR
1	A	45	LYS
1	A	51	PRO
1	A	52	TYR
1	A	64	THR
1	A	67	LEU
1	A	74	VAL
1	A	84	CYS
1	A	97	ILE
1	A	103	LYS
1	A	106	ARG
1	A	107	GLU
1	A	110	LEU
1	A	111	TYR
1	A	113	CYS
1	A	161	MET
1	A	168	ASP
1	A	172	VAL
1	A	184	PHE
1	A	197	LEU
1	A	207	THR
1	A	208	THR
1	A	221	GLN
1	A	223	LEU
1	A	229	ASN
1	A	231	ILE
1	A	252	ASP
1	A	264	TYR
1	A	267	LEU
1	A	271	VAL
1	A	272	LEU
1	A	277	SER
1	A	283	LYS
1	A	299	MET
1	A	303	THR
1	A	305	CYS
1	A	307	VAL
1	A	319	VAL
1	A	325	ILE

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Mol	Chain	Res	Type
1	A	329	LYS
1	A	333	ASN
1	A	343	ASN
1	A	351	GLU
1	A	352	LEU
1	A	356	GLU
1	A	358	LEU
1	A	370	LYS
1	A	374	VAL
1	A	389	VAL
1	A	400	ILE
1	A	403	LEU
1	A	409	LYS
1	A	415	LYS
1	A	418	ILE
1	A	424	LEU
1	A	439	ASN
1	A	440	LEU
1	A	449	LEU
1	A	451	ILE
1	A	452	GLN
1	A	457	ARG
1	A	460	LEU
1	A	469	LEU
1	A	474	GLU
1	A	479	VAL
1	A	498	MET
1	A	499	ILE
1	A	500	ASP
1	A	512	LYS
1	A	517	ARG
1	A	519	SER
1	A	523	VAL
1	A	526	LEU
1	A	528	ASP
1	A	531	TYR
1	A	542	GLN
1	A	553	PHE
1	A	579	LEU
1	A	583	LEU
1	A	591	ILE
1	A	593	SER

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Mol	Chain	Res	Type
1	A	598	THR
1	A	601	MET
1	A	610	LEU
1	A	629	GLN
1	A	642	GLU
1	A	647	LYS
1	A	648	THR
1	A	672	VAL
1	A	676	ASP
1	A	680	ASN
1	A	695	GLU
1	A	698	ASP
1	A	702	THR
1	A	704	VAL
1	A	712	LEU
1	A	715	GLU
1	A	719	LYS
1	A	720	SER
1	A	731	ILE
1	A	739	MET
1	A	749	THR
1	A	754	ASN
1	A	759	MET
1	A	761	ASP
1	A	765	LEU
1	A	777	MET
1	A	781	TRP
1	A	782	ASP
1	A	791	THR
1	A	799	SER
1	A	806	ILE
1	A	829	GLN
1	A	834	LYS
1	A	837	GLU
1	A	843	MET
1	A	848	VAL
1	A	852	ILE
1	A	856	THR
1	A	865	HIS
1	A	866	LEU
1	A	870	ILE
1	A	873	LEU

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Mol	Chain	Res	Type
1	A	881	MET
1	A	894	VAL
1	A	895	LEU
1	A	898	SER
1	A	902	LEU
1	A	913	LEU
1	A	915	ASN
1	A	936	CYS
1	A	943	ASN
1	A	949	HIS
1	A	951	THR
1	A	952	LEU
1	A	970	LYS
1	A	971	VAL
1	A	972	ILE
1	A	975	GLU
1	A	978	SER
1	A	981	GLU
1	A	993	VAL
1	A	1000	LEU
1	A	1001	GLU
1	A	1008	LEU
1	A	1014	PHE
1	A	1020	LEU
1	A	1025	VAL
1	A	1031	LEU
1	A	1038	VAL
1	A	1042	SER
1	A	1049	ARG
1	A	1050	GLU
1	A	1052	CYS
1	A	1053	CYS
1	A	1059	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	157	GLN
1	A	221	GLN
1	A	454	GLN
1	A	538	ASN

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Mol	Chain	Res	Type
1	A	569	GLN
1	A	611	GLN
1	A	688	ASN
1	A	689	HIS
1	A	696	GLN
1	A	900	GLN
1	A	958	HIS
1	A	962	ASN

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LEU	A	1201	-	6,8,8	0.97	1 (16%)	5,10,10	1.41	1 (20%)
2	LEU	A	1202	-	6,8,8	0.98	1 (16%)	5,10,10	1.56	1 (20%)
3	PO4	A	1203	-	4,4,4	0.87	0	6,6,6	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LEU	A	1201	-	-	1/8/8/8	-
2	LEU	A	1202	-	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1202	LEU	OXT-C	-2.12	1.23	1.30
2	A	1201	LEU	OXT-C	-2.08	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1202	LEU	OXT-C-O	-3.42	116.33	124.08
2	A	1201	LEU	OXT-C-O	-3.09	117.07	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	LEU	N-CA-CB-CG
2	A	1202	LEU	O-C-CA-N
2	A	1202	LEU	OXT-C-CA-N
2	A	1202	LEU	OXT-C-CA-CB
2	A	1202	LEU	O-C-CA-CB

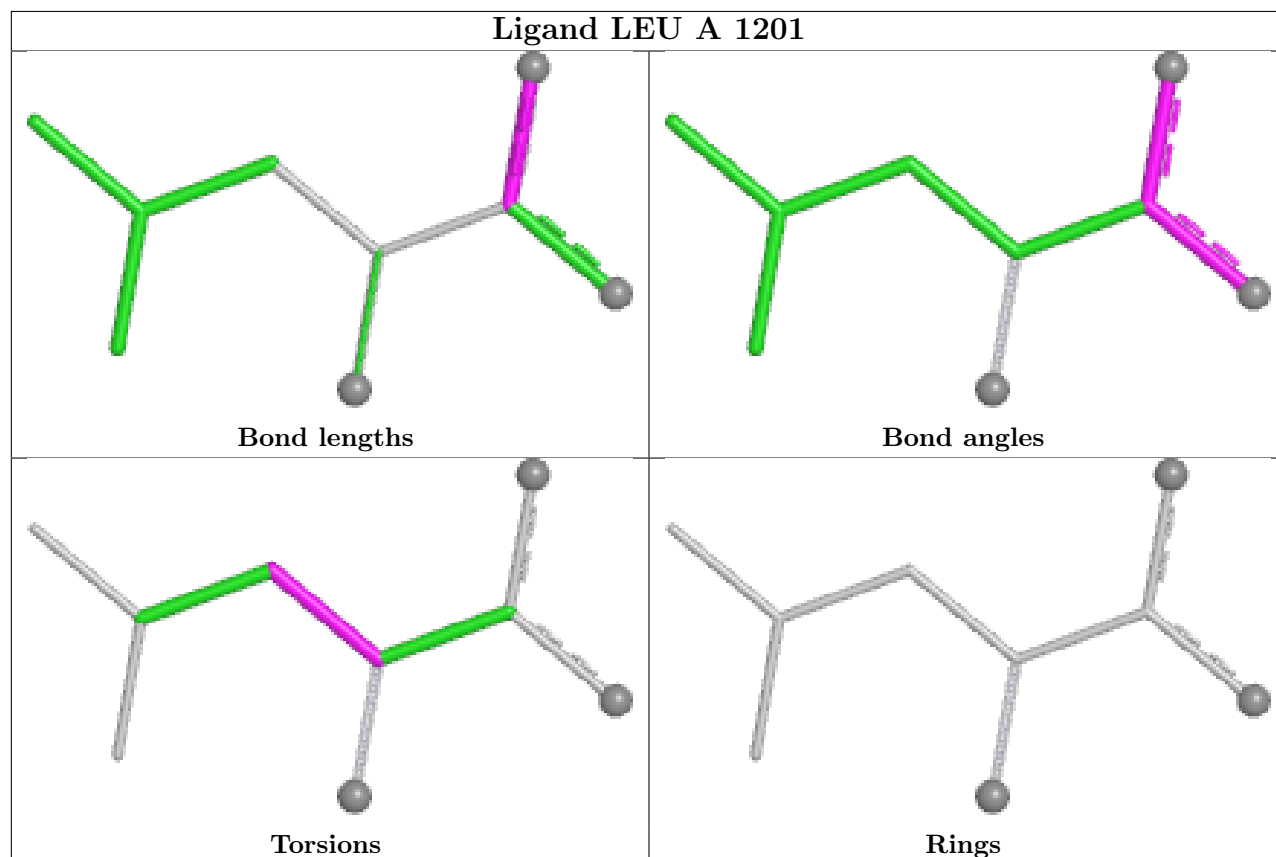
There are no ring outliers.

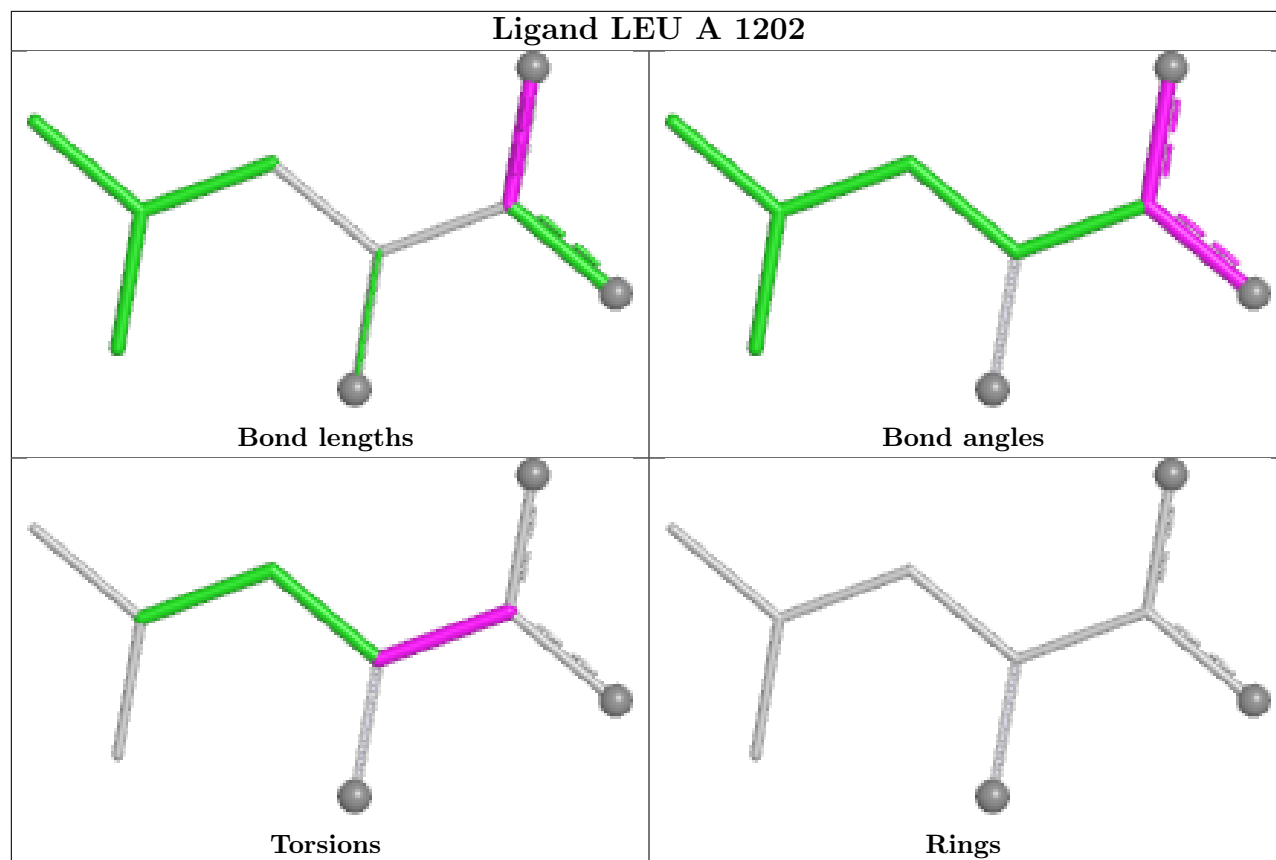
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1202	LEU	4	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1002/1188 (84%)	0.51	83 (8%) 17 13	10, 38, 143, 216	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	ASN	7.3
1	A	996	ILE	6.8
1	A	841	GLU	6.2
1	A	959	PHE	5.3
1	A	1054	PRO	5.2
1	A	417	GLY	5.0
1	A	946	PRO	4.9
1	A	1005	PRO	4.8
1	A	463	ALA	4.6
1	A	1053	CYS	4.5
1	A	421	ASP	4.4
1	A	972	ILE	4.2
1	A	390	THR	3.9
1	A	454	GLN	3.8
1	A	954	VAL	3.8
1	A	995	MET	3.8
1	A	961	ALA	3.8
1	A	743	LEU	3.8
1	A	909	LEU	3.7
1	A	990	MET	3.7
1	A	57	GLY	3.7
1	A	948	GLN	3.5
1	A	1052	CYS	3.4
1	A	1010	LEU	3.4
1	A	527	CYS	3.3
1	A	456	ASP	3.2
1	A	379	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1007	ILE	3.2
1	A	414	ALA	3.2
1	A	962	ASN	3.1
1	A	109	GLU	3.1
1	A	448	GLU	3.1
1	A	293	THR	3.1
1	A	1048	ILE	2.9
1	A	670	LEU	2.9
1	A	466	LYS	2.9
1	A	1011	GLN	2.9
1	A	958	HIS	2.8
1	A	1008	LEU	2.8
1	A	703	ALA	2.8
1	A	611	GLN	2.7
1	A	204	SER	2.7
1	A	1061	PHE	2.7
1	A	655	LEU	2.7
1	A	992	PHE	2.6
1	A	1055	GLY	2.6
1	A	960	GLU	2.5
1	A	460	LEU	2.5
1	A	976	LEU	2.5
1	A	999	ASN	2.5
1	A	524	VAL	2.5
1	A	899	SER	2.4
1	A	942	LYS	2.4
1	A	208	THR	2.4
1	A	87	PRO	2.4
1	A	97	ILE	2.4
1	A	704	VAL	2.4
1	A	294	LEU	2.4
1	A	874	LEU	2.3
1	A	217	PHE	2.3
1	A	991	PRO	2.3
1	A	947	TRP	2.2
1	A	37	LEU	2.2
1	A	973	ALA	2.2
1	A	944	TYR	2.2
1	A	464	LYS	2.2
1	A	916	TYR	2.2
1	A	764	ILE	2.2
1	A	725	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	877	PRO	2.1
1	A	1042	SER	2.1
1	A	389	VAL	2.1
1	A	695	GLU	2.1
1	A	971	VAL	2.1
1	A	369	TYR	2.1
1	A	36	ASN	2.0
1	A	110	LEU	2.0
1	A	231	ILE	2.0
1	A	363	SER	2.0
1	A	292	ALA	2.0
1	A	416	TYR	2.0
1	A	528	ASP	2.0
1	A	627	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

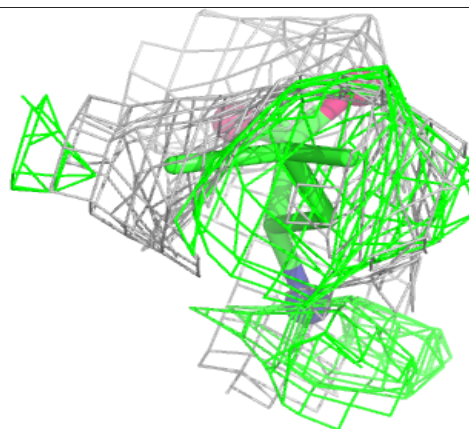
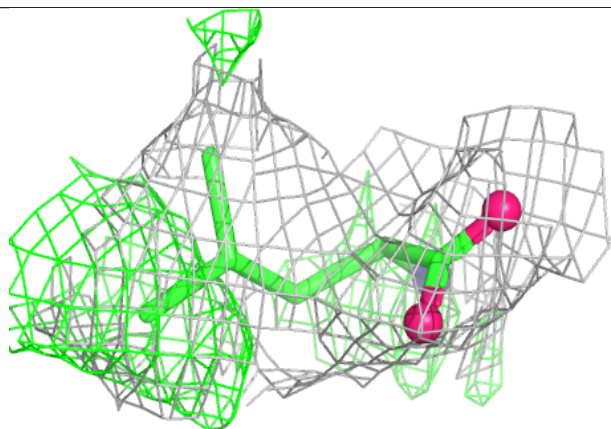
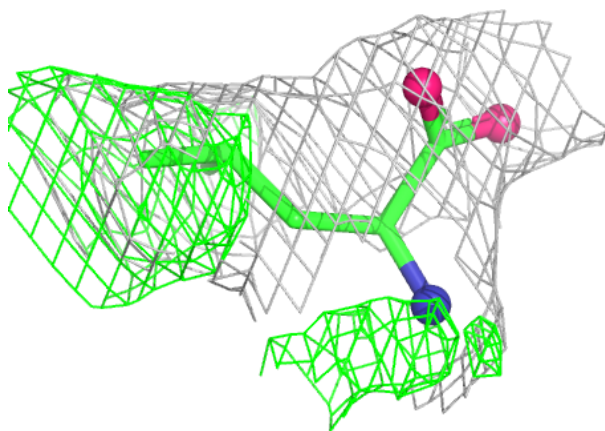
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LEU	A	1202	9/9	0.66	0.29	11,21,50,54	0
3	PO4	A	1203	5/5	0.74	0.16	87,91,93,100	0
2	LEU	A	1201	9/9	0.96	0.11	10,23,29,31	0

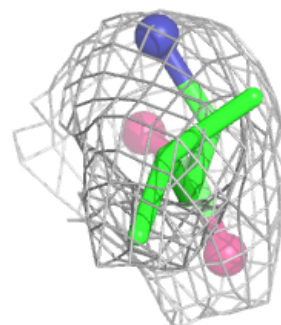
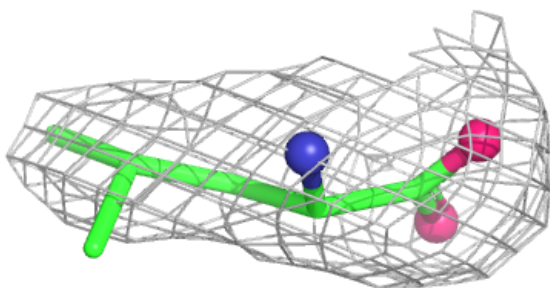
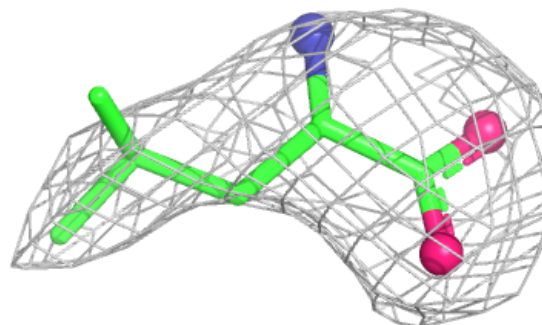
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LEU A 1202:

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

**Electron density around LEU A 1201:**

$2mF_o-DF_c$ (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.