



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 09:05 PM JST

PDB ID : 6KQY
Title : Crystal structure of human leucyl-tRNA synthetase, Leucine-bound form
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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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

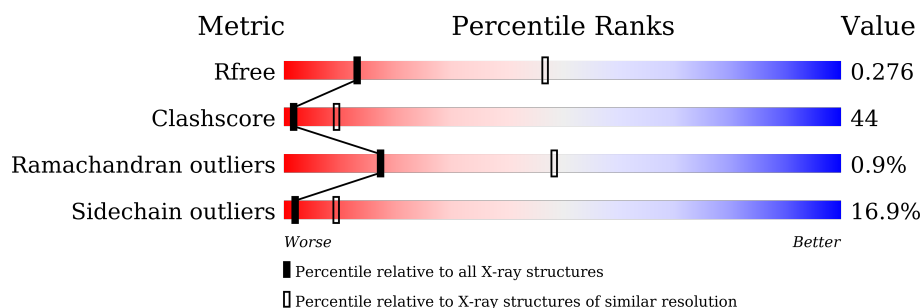
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 $\leq 5\%$.

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.

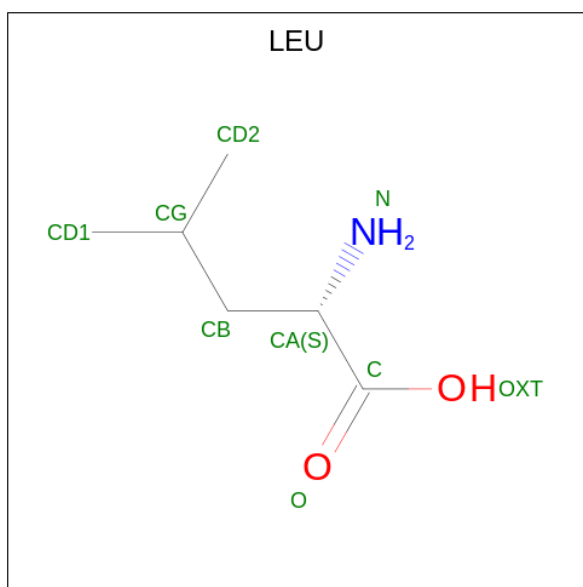
- Molecule 1 is a protein called Leucine-tRNA ligase, cytoplasmic.

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:

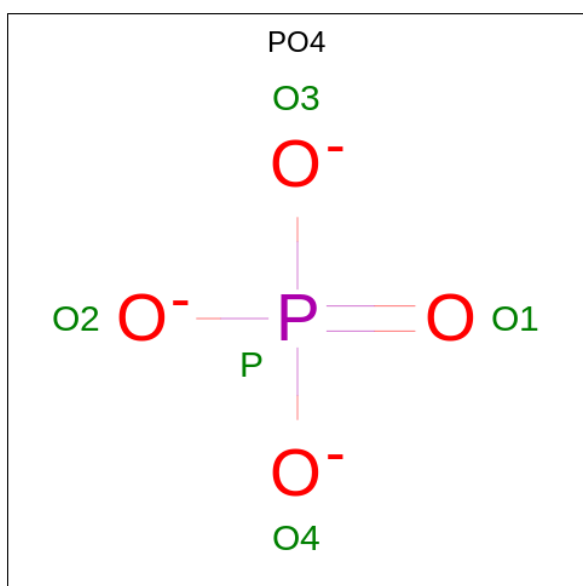
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9P2J5
A	-10	ARG	-	expression tag	UNP Q9P2J5
A	-9	GLY	-	expression tag	UNP Q9P2J5
A	-8	SER	-	expression tag	UNP Q9P2J5
A	-7	HIS	-	expression tag	UNP Q9P2J5
A	-6	HIS	-	expression tag	UNP Q9P2J5
A	-5	HIS	-	expression 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 (three-letter code: 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 (three-letter code: PO4) (formula: O_4P).



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

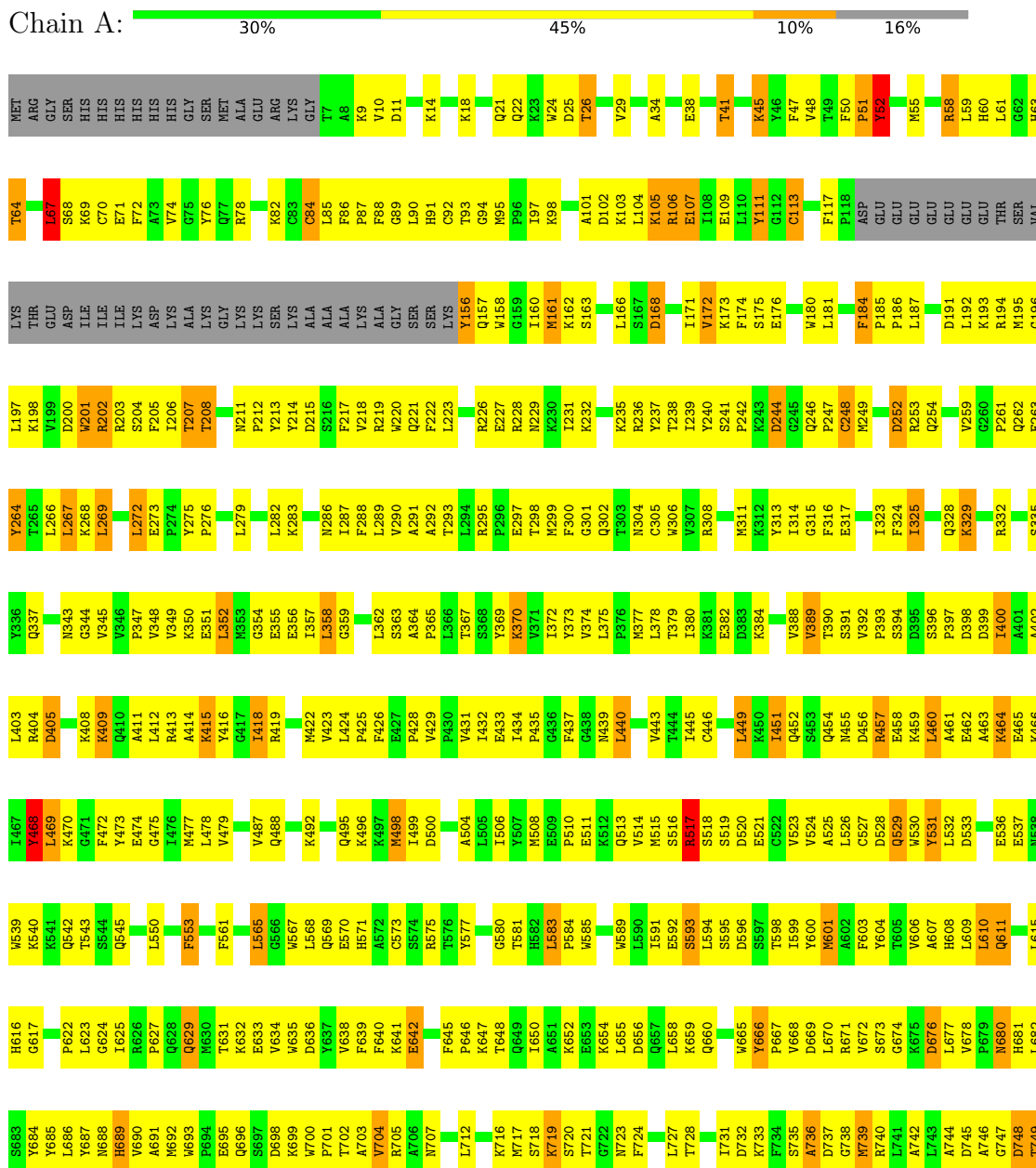
- Molecule 4 is water.

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

3 Residue-property plots

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

- Molecule 1: Leucine-tRNA ligase, cytoplasmic





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 – 2.83	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.76-3.30) 94.7 (49.76-2.83)	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 0.249 , 0.276	Depositor DCC
R_{free} test set	1937 reflections (3.46%)	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)	0.08 , 10.9	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	0.53	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	0.60	0/8288	0.79	9/11203 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1041	ALA	N-CA-CB	6.66	119.42	110.10
1	A	52	TYR	CA-CB-CG	6.27	125.32	113.40
1	A	565	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	67	LEU	CA-CB-CG	6.19	129.55	115.30
1	A	1041	ALA	CB-CA-C	5.81	118.81	110.10
1	A	59	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	A	1021	MET	C-N-CA	5.62	135.74	121.70
1	A	67	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	809	ASP	CB-CG-OD2	5.12	122.91	118.30

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	708	6
2	A	18	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
4	A	447	0	0	77	0
All	All	8558	0	8066	708	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 44.

All (708) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:308:ARG:HB3	1:A:311:MET:HE3	1.59	0.82
1:A:958:HIS:CE1	1:A:962:ASN:CG	2.51	0.82
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: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: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:299:MET:HE2	1:A:299:MET:HA	1.68	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:638:VAL:O	1:A:659:LYS:NZ	2.18	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:731:ILE:HG12	1:A:739:MET:HE1	1.71	0.72
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: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:384:LYS:NZ	2:A:1202:LEU:HD21	2.07	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1020:LEU:C	1:A:1022:GLU:H	1.97	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:607:ALA:O	1:A:611:GLN:CG	2.45	0.65
1:A:295:ARG:O	1:A:298:THR:OG1	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:405:ASP:CG	1:A:454:GLN:HB2	2.18	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: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
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:466:LYS:C	1:A:468:TYR:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:384:LYS:HZ1	2:A:1202:LEU:HD21	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:937:THR:C	1:A:938:ILE:HD13	2.25	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:LYS:HZ1	1:A:748:ASP:HA	1.73	0.53
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: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:606:VAL:HB	1:A:610:LEU:HD12	1.90	0.53
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: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:746:ALA:O	1:A:753:ALA:HB1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:VAL:O	1:A:350:LYS:HG3	2.09	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:1029:ASN:C	1:A:1031:LEU:H	2.13	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: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:367:THR:C	1:A:369:TYR:H	2.13	0.51
1:A:609:LEU:HB2	1:A:658:LEU:HD21	1.93	0.51
1:A:205:PHE:HB3	1:A:611:GLN:NE2	1.99	0.51
1:A:959:PHE:C	1:A:961:ALA:H	2.14	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:639:PHE:C	1:A:659:LYS:HZ1	2.15	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
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: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:78:ARG:HD3	1:A:881:MET:HE2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:LYS:NZ	4:A:1371:HOH:O	2.43	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
1:A:748:ASP:OD2	1:A:818:LYS:N	2.45	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:409:LYS:HG3	1:A:411:ALA:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:599:ILE:HD13	1:A:692:MET:HE1	1.96	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:745:ASP:C	1:A:747:GLY:H	2.17	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:335:SER:HB2	1:A:344:GLY:C	2.34	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
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: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:565:LEU:C	1:A:567:TRP:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:745:ASP:HB3	1:A:759:MET:HE1	1.97	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:594:LEU:HD21	1:A:681:HIS:HB2	1.98	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:397:PRO:O	1:A:398:ASP:C	2.55	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
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:195:MET:CE	1:A:197:LEU:HD21	2.47	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:638:VAL:C	1:A:659:LYS:HZ3	2.14	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:161:MET:HE3	1:A:180:TRP:CZ2	2.52	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:1029:ASN:O	1:A:1031:LEU:N	2.52	0.43
1:A:415:LYS:HG2	1:A:416:TYR:CZ	2.54	0.43
1:A:263:GLU:HB2	1:A:508:MET:HE1	2.01	0.43
1:A:938:ILE:O	1:A:1038:VAL:HG23	2.18	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:60:HIS:CE1	1:A:63:HIS:CE1	3.06	0.43
1:A:806:ILE:O	1:A:807:LYS:C	2.57	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: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:735:SER:O	1:A:737:ASP:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:CD1	1:A:357:ILE:HD11	2.36	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
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:600:TYR:CD1	1:A:600:TYR:C	2.93	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:55:MET:CE	1:A:55:MET:HA	2.50	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: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: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:304:ASN:H	1:A:391:SER:HG	1.65	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:466:LYS:C	1:A:468:TYR:N	2.72	0.41
1:A:770:TRP:CH2	1:A:855:GLN:HG2	2.55	0.41
1:A:777:MET:HE3	1:A:777:MET:HB2	1.93	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: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: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:781:TRP:C	1:A:783:SER:H	2.23	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: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:671:ARG:HG2	1:A:672:VAL:N	2.35	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: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: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
1:A:1003:MET:HE3	1:A:1007:ILE:HG13	2.03	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

5.3.1 Protein backbone

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%)	17	48

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 ⓘ

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%)	733 (83%)	150 (17%)	2	9

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	26	THR
1	A	41	THR
1	A	45	LYS
1	A	51	PRO
1	A	52	TYR
1	A	58	ARG
1	A	64	THR
1	A	67	LEU
1	A	84	CYS

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Mol	Chain	Res	Type
1	A	105	LYS
1	A	106	ARG
1	A	107	GLU
1	A	111	TYR
1	A	113	CYS
1	A	156	TYR
1	A	161	MET
1	A	168	ASP
1	A	172	VAL
1	A	173	LYS
1	A	176	GLU
1	A	184	PHE
1	A	201	TRP
1	A	202	ARG
1	A	207	THR
1	A	208	THR
1	A	226	ARG
1	A	229	ASN
1	A	244	ASP
1	A	248	CYS
1	A	252	ASP
1	A	264	TYR
1	A	267	LEU
1	A	269	LEU
1	A	272	LEU
1	A	283	LYS
1	A	305	CYS
1	A	325	ILE
1	A	329	LYS
1	A	343	ASN
1	A	352	LEU
1	A	356	GLU
1	A	358	LEU
1	A	370	LYS
1	A	389	VAL
1	A	400	ILE
1	A	403	LEU
1	A	405	ASP
1	A	409	LYS
1	A	415	LYS
1	A	418	ILE
1	A	439	ASN

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Mol	Chain	Res	Type
1	A	440	LEU
1	A	449	LEU
1	A	451	ILE
1	A	457	ARG
1	A	460	LEU
1	A	464	LYS
1	A	468	TYR
1	A	469	LEU
1	A	479	VAL
1	A	492	LYS
1	A	498	MET
1	A	500	ASP
1	A	517	ARG
1	A	519	SER
1	A	520	ASP
1	A	526	LEU
1	A	528	ASP
1	A	529	GLN
1	A	531	TYR
1	A	542	GLN
1	A	553	PHE
1	A	583	LEU
1	A	593	SER
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	656	ASP
1	A	666	TYR
1	A	676	ASP
1	A	680	ASN
1	A	689	HIS
1	A	695	GLU
1	A	698	ASP
1	A	702	THR
1	A	704	VAL
1	A	712	LEU
1	A	719	LYS
1	A	720	SER

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Mol	Chain	Res	Type
1	A	739	MET
1	A	748	ASP
1	A	749	THR
1	A	754	ASN
1	A	755	PHE
1	A	759	MET
1	A	761	ASP
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	836	ARG
1	A	837	GLU
1	A	852	ILE
1	A	856	THR
1	A	865	HIS
1	A	866	LEU
1	A	869	HIS
1	A	873	LEU
1	A	894	VAL
1	A	895	LEU
1	A	898	SER
1	A	902	LEU
1	A	913	LEU
1	A	914	LYS
1	A	915	ASN
1	A	936	CYS
1	A	942	LYS
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	985	TYR

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Mol	Chain	Res	Type
1	A	993	VAL
1	A	1000	LEU
1	A	1001	GLU
1	A	1014	PHE
1	A	1020	LEU
1	A	1025	VAL
1	A	1031	LEU
1	A	1040	PHE
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 (11) 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	569	GLN
1	A	611	GLN
1	A	688	ASN
1	A	689	HIS
1	A	696	GLN
1	A	958	HIS
1	A	962	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
3	PO4	A	1203	-	4,4,4	0.82	0	6,6,6	0.44	0
2	LEU	A	1202	-	5,8,8	0.33	0	6,10,10	0.47	0
2	LEU	A	1201	-	5,8,8	0.45	0	6,10,10	0.47	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	1202	-	-	0/4/8/8	-
2	LEU	A	1201	-	-	1/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

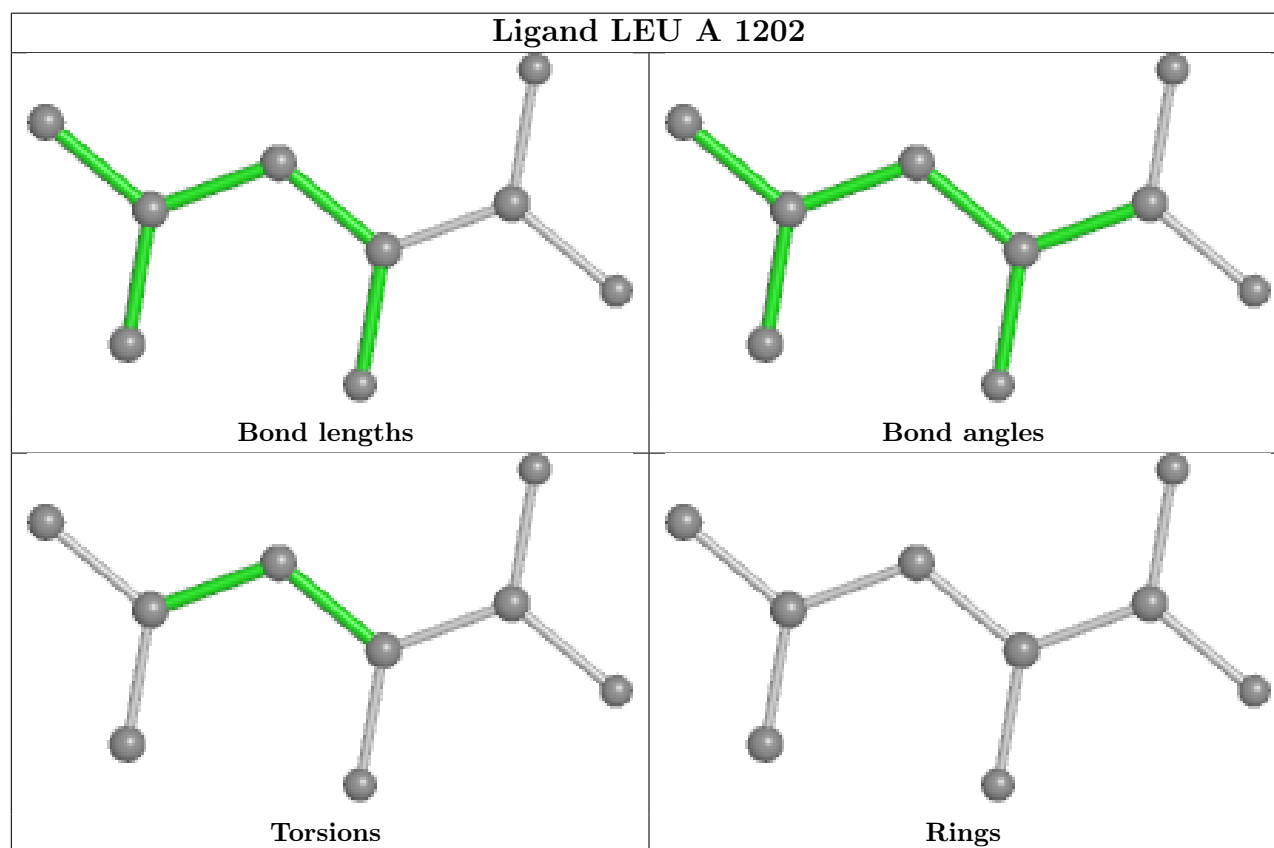
Mol	Chain	Res	Type	Atoms
2	A	1201	LEU	N-CA-CB-CG

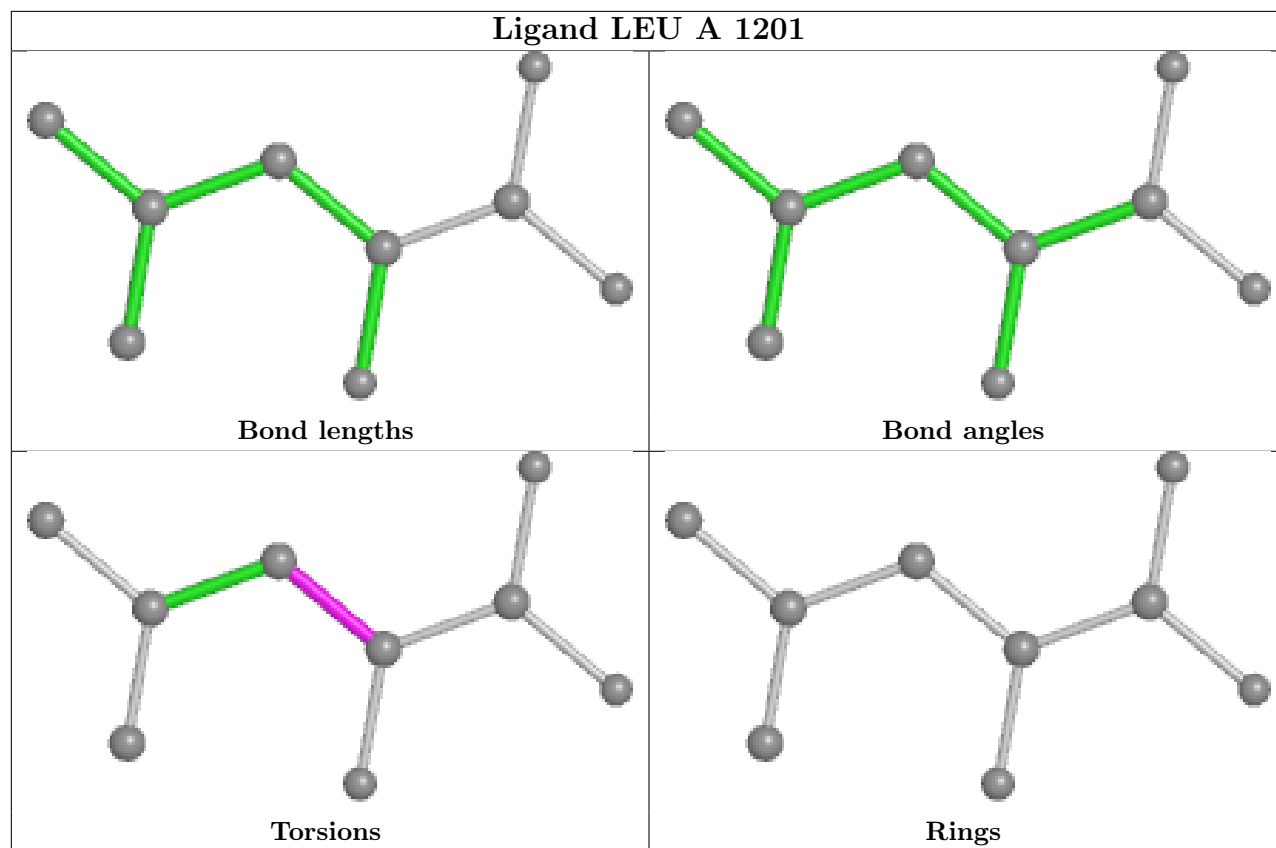
There are no ring outliers.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

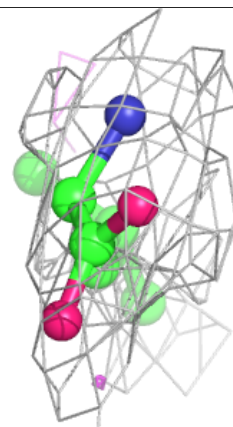
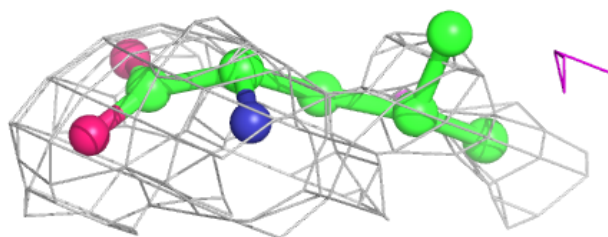
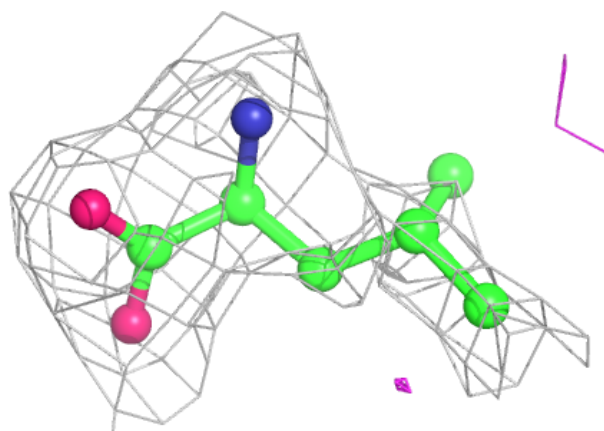
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

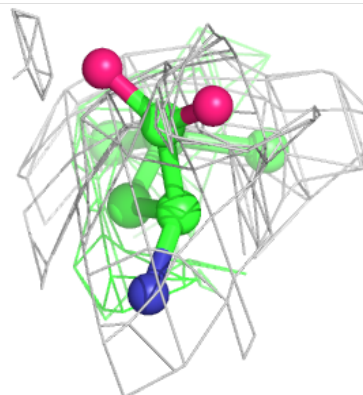
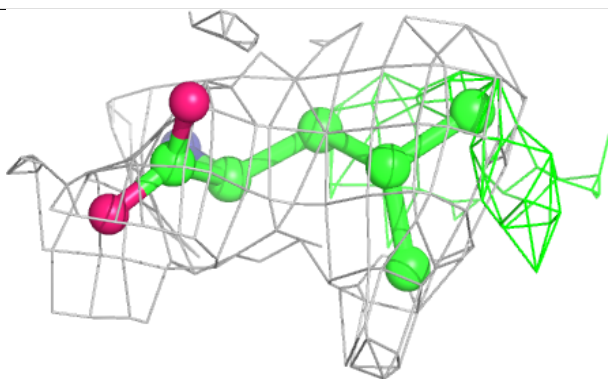
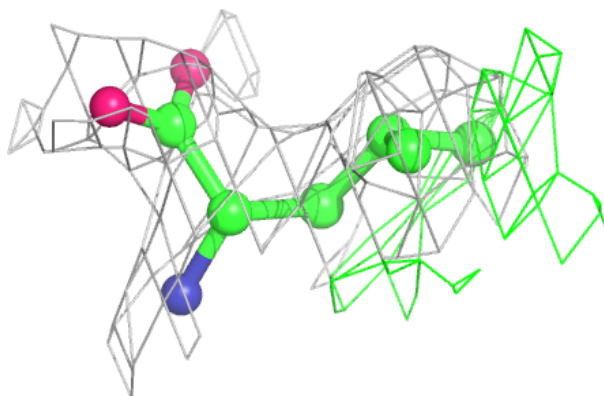
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LEU A 1201:

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

**Electron density around LEU A 1202:**

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.