Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 02:06 AM JST

PDB ID	:	6KIE
Title	:	Crystal structure of human leucyl-tRNA synthetase, Leu-AMS-bound form
Authors	:	Kim, S.; Son, J.; Kim, S.; Hwang, K.Y.
Deposited on	:	2019-07-18
Resolution	:	3.15 Å(reported)

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

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

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

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

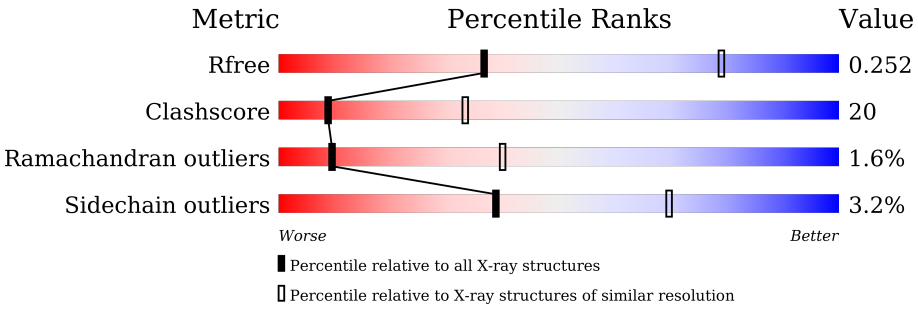
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	1073	57% 34% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1102	-	X	-	-
2	PO4	A	1103	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8233 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.

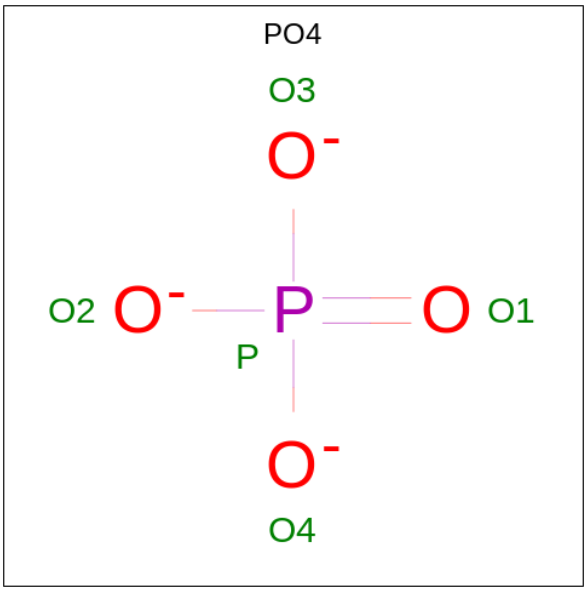
- Molecule 1 is a protein called Leucine–tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1004	8103	5213	1346	1491	53	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

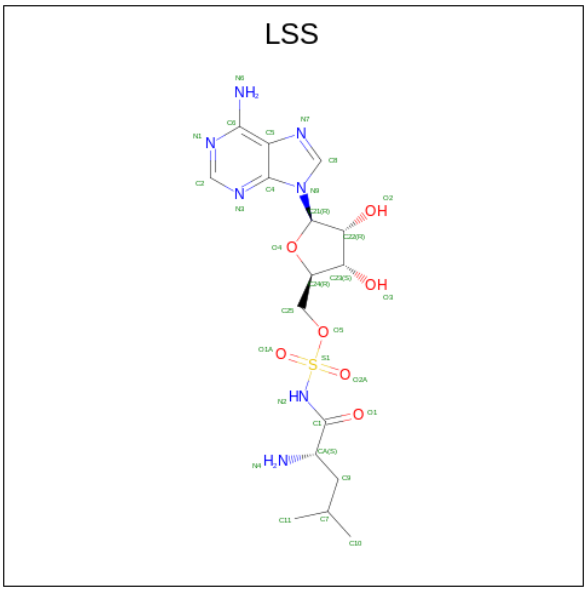
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9P2J5
A	-10	ARG	-	expression tag	UNP Q9P2J5
A	-9	GLY	-	expression tag	UNP Q9P2J5
A	-8	SER	-	expression tag	UNP Q9P2J5
A	-7	HIS	-	expression tag	UNP Q9P2J5
A	-6	HIS	-	expression tag	UNP Q9P2J5
A	-5	HIS	-	expression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



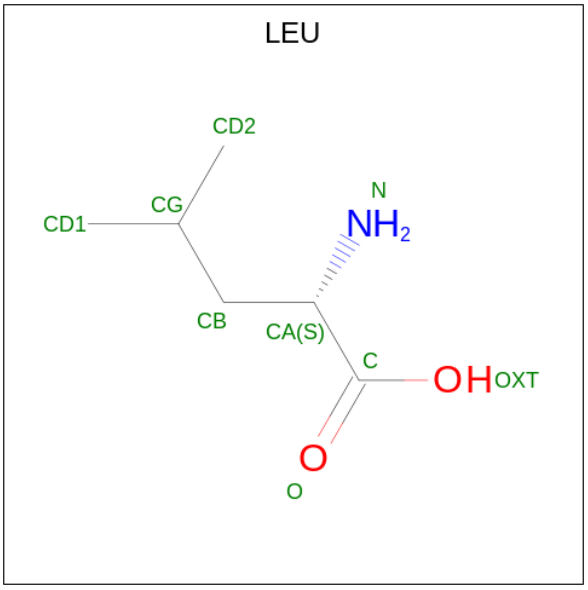
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0

- Molecule 3 is 5'-O-(L-leucylsulfamoyl)adenosine (three-letter code: LSS) (formula: $C_{16}H_{25}N_7O_7S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	16	7	7	1		

- Molecule 4 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



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

- Molecule 5 is water.

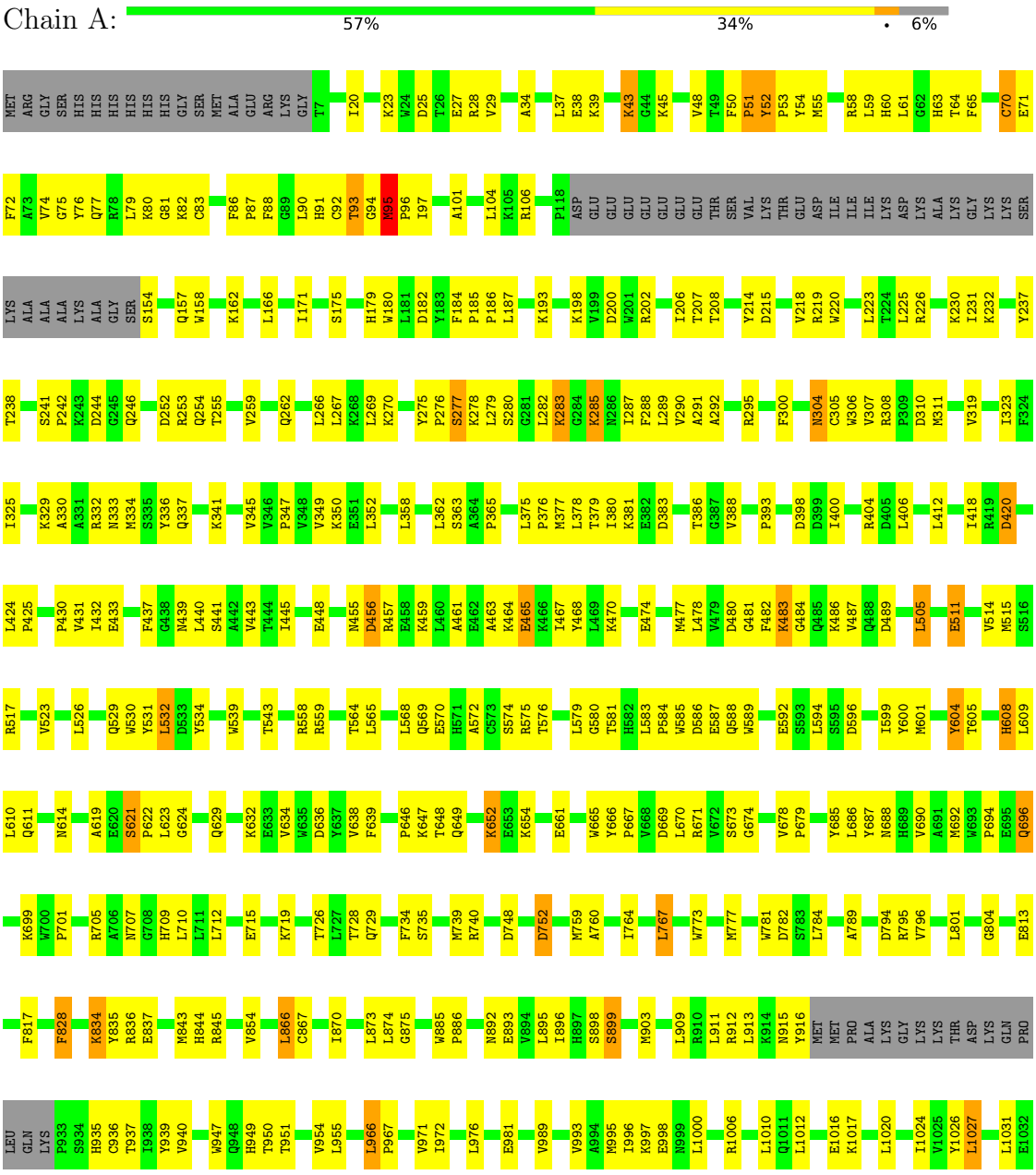
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		

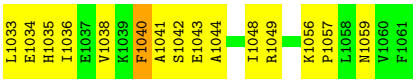
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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

Chain A:




L1033
E1034
H1035
I1036
E1037
V1038
K1039
F1040
A1041
S1042
E1043
A1044
I1048
R1049
K1056
P1057
L1058
N1059
V1060
F1061

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	138.77Å 138.77Å 448.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.85 – 3.15 46.85 – 3.15	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.85-3.15) 96.7 (46.85-3.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.229 , 0.251 0.229 , 0.252	Depositor DCC
R_{free} test set	1901 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8233	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.73	5/8303 (0.1%)	0.86	12/11222 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	MET	C-N	9.41	1.52	1.34
1	A	867	CYS	CB-SG	-6.01	1.72	1.82
1	A	305	CYS	CB-SG	-5.45	1.73	1.81
1	A	52	TYR	CE1-CZ	-5.07	1.31	1.38
1	A	752	ASP	CB-CG	5.00	1.62	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1027	LEU	CA-CB-CG	-9.25	94.02	115.30
1	A	59	LEU	CA-CB-CG	-6.45	100.48	115.30
1	A	966	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	767	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	532	LEU	CA-CB-CG	-5.87	101.80	115.30
1	A	1000	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	505	LEU	CA-CB-CG	5.79	128.61	115.30
1	A	285	LYS	CD-CE-NZ	5.42	124.16	111.70
1	A	358	LEU	CA-CB-CG	-5.34	103.01	115.30
1	A	801	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	193	LYS	CA-CB-CG	5.26	124.96	113.40
1	A	363	SER	C-N-CA	-5.08	109.00	121.70

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	8103	0	8064	331	0
2	A	15	0	0	1	0
3	A	31	0	21	6	0
4	A	9	0	10	0	0
5	A	75	0	0	11	0
All	All	8233	0	8095	331	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (331) 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:481:GLY:H	1:A:483:LYS:HE2	1.32	0.93
1:A:481:GLY:N	1:A:483:LYS:HE2	1.84	0.92
1:A:966:LEU:HD23	1:A:997:LYS:HE2	1.52	0.91
1:A:267:LEU:HD23	1:A:365:PRO:HG2	1.52	0.91
1:A:154:SER:N	5:A:1201:HOH:O	2.05	0.88
1:A:936:CYS:SG	1:A:937:THR:N	2.51	0.83
1:A:1027:LEU:O	1:A:1031:LEU:HB2	1.83	0.79
1:A:269:LEU:HB3	1:A:362:LEU:HD22	1.66	0.78
1:A:97:ILE:HD12	1:A:97:ILE:H	1.50	0.77
1:A:280:SER:O	1:A:283:LYS:HG2	1.85	0.76
1:A:92:CYS:HB2	1:A:208:THR:HG23	1.67	0.75
1:A:282:LEU:HD13	1:A:323:ILE:HG13	1.67	0.75
1:A:53:PRO:HA	3:A:1104:LSS:HN2	1.50	0.75
1:A:52:TYR:HE2	1:A:207:THR:HG21	1.52	0.74
1:A:333:ASN:OD1	1:A:523:VAL:HB	1.87	0.74
1:A:481:GLY:CA	1:A:483:LYS:HE2	2.17	0.74
1:A:282:LEU:HB3	1:A:285:LYS:HE2	1.70	0.72
1:A:767:LEU:HD22	1:A:866:LEU:HD12	1.69	0.72
1:A:481:GLY:H	1:A:483:LYS:CE	2.02	0.71
1:A:277:SER:OG	5:A:1202:HOH:O	2.09	0.70
1:A:673:SER:OG	1:A:674:GLY:N	2.23	0.70
1:A:543:THR:HG21	1:A:687:TYR:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TYR:CE2	1:A:207:THR:HG21	2.26	0.69
1:A:939:TYR:CD1	1:A:1044:ALA:HB2	2.27	0.69
1:A:796:VAL:HG23	1:A:895:LEU:HD22	1.75	0.68
1:A:92:CYS:C	1:A:94:GLY:H	1.97	0.68
1:A:456:ASP:HB3	1:A:459:LYS:HD3	1.76	0.68
1:A:543:THR:HA	1:A:690:VAL:HG21	1.77	0.67
1:A:43:LYS:HG3	1:A:82:LYS:HG2	1.77	0.67
1:A:804:GLY:HA3	1:A:828:PHE:HE1	1.61	0.66
1:A:967:PRO:HB2	1:A:971:VAL:HB	1.77	0.66
1:A:393:PRO:O	1:A:400:ILE:HB	1.96	0.65
1:A:278:LYS:HE2	1:A:350:LYS:HE3	1.77	0.65
1:A:50:PHE:CZ	3:A:1104:LSS:H24	2.32	0.65
1:A:534:TYR:HB2	1:A:569:GLN:O	1.97	0.65
1:A:955:LEU:HD11	1:A:993:VAL:HG13	1.79	0.64
1:A:74:VAL:HG23	1:A:198:LYS:HD2	1.80	0.64
1:A:588:GLN:NE2	5:A:1204:HOH:O	2.20	0.64
1:A:95:MET:N	1:A:96:PRO:CD	2.60	0.64
1:A:53:PRO:HA	3:A:1104:LSS:N2	2.12	0.63
1:A:1017:LYS:O	1:A:1020:LEU:HB2	1.98	0.63
1:A:936:CYS:HB3	1:A:1036:ILE:HG12	1.80	0.63
1:A:246:GLN:HB3	1:A:576:THR:HG22	1.80	0.63
1:A:940:VAL:HG22	1:A:1057:PRO:HB3	1.79	0.63
1:A:225:LEU:HB3	1:A:231:ILE:HG13	1.79	0.63
1:A:52:TYR:CD1	1:A:600:TYR:CZ	2.87	0.63
1:A:266:LEU:HD11	1:A:290:VAL:HG22	1.82	0.61
1:A:283:LYS:HA	1:A:283:LYS:HZ2	1.65	0.61
1:A:1016:GLU:O	1:A:1020:LEU:HG	1.99	0.61
1:A:280:SER:O	1:A:283:LYS:NZ	2.32	0.61
1:A:276:PRO:O	1:A:278:LYS:N	2.33	0.60
1:A:232:LYS:HB2	1:A:531:TYR:CZ	2.36	0.60
1:A:27:GLU:HG3	1:A:29:VAL:HG13	1.83	0.60
1:A:337:GLN:HA	1:A:526:LEU:HB3	1.84	0.60
1:A:610:LEU:O	1:A:622:PRO:HD2	2.01	0.60
1:A:308:ARG:HD2	1:A:311:MET:HE2	1.84	0.60
1:A:50:PHE:CD1	1:A:51:PRO:HD2	2.37	0.59
1:A:242:PRO:HG2	1:A:332:ARG:HH21	1.66	0.59
1:A:270:LYS:HB2	1:A:288:PHE:HE1	1.67	0.59
1:A:583:LEU:HD11	1:A:585:TRP:CZ2	2.36	0.59
1:A:94:GLY:HA3	1:A:96:PRO:HD2	1.83	0.59
1:A:455:ASN:O	1:A:457:ARG:N	2.36	0.59
1:A:219:ARG:O	1:A:223:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLN:HB2	1:A:511:GLU:HG2	1.85	0.59
1:A:586:ASP:HB3	1:A:589:TRP:HD1	1.67	0.58
1:A:647:LYS:HE2	1:A:647:LYS:O	2.04	0.58
1:A:241:SER:HB3	1:A:244:ASP:HB2	1.84	0.58
1:A:789:ALA:HB2	1:A:844:HIS:CG	2.38	0.58
1:A:350:LYS:NZ	5:A:1207:HOH:O	2.37	0.58
1:A:1056:LYS:NZ	1:A:1056:LYS:HB3	2.19	0.58
1:A:58:ARG:NH2	1:A:728:THR:HG21	2.19	0.57
1:A:259:VAL:HG13	1:A:511:GLU:HB2	1.85	0.57
1:A:430:PRO:HB3	1:A:439:ASN:HB3	1.86	0.57
1:A:634:VAL:HA	1:A:646:PRO:HG3	1.85	0.57
1:A:678:VAL:HB	1:A:679:PRO:HD3	1.87	0.57
1:A:39:LYS:N	1:A:39:LYS:HE2	2.19	0.56
1:A:226:ARG:HD2	1:A:585:TRP:CE2	2.40	0.56
1:A:376:PRO:HD3	1:A:418:ILE:HD11	1.88	0.56
1:A:482:PHE:O	1:A:484:GLY:N	2.38	0.56
1:A:837:GLU:HG3	1:A:1026:TYR:CE1	2.41	0.56
1:A:61:LEU:O	1:A:64:THR:N	2.39	0.56
1:A:568:LEU:HD23	1:A:687:TYR:HE2	1.70	0.56
1:A:282:LEU:HD11	1:A:349:VAL:HG21	1.87	0.55
1:A:76:TYR:CE2	1:A:813:GLU:HG3	2.41	0.55
1:A:295:ARG:HD2	1:A:468:TYR:CZ	2.39	0.55
1:A:76:TYR:HE2	1:A:813:GLU:HG3	1.71	0.55
1:A:275:TYR:HB3	1:A:279:LEU:HB2	1.88	0.55
1:A:445:ILE:HD13	1:A:467:ILE:HB	1.88	0.55
1:A:632:LYS:NZ	1:A:636:ASP:OD2	2.38	0.55
1:A:52:TYR:HD1	1:A:600:TYR:CZ	2.24	0.55
1:A:794:ASP:OD1	1:A:835:TYR:HE1	1.89	0.55
1:A:92:CYS:C	1:A:94:GLY:N	2.60	0.55
1:A:225:LEU:HD22	1:A:230:LYS:HB2	1.89	0.55
1:A:226:ARG:HD2	1:A:585:TRP:CZ2	2.41	0.55
1:A:951:THR:HG22	1:A:976:LEU:HD22	1.87	0.55
1:A:592:GLU:OE2	1:A:594:LEU:HB2	2.06	0.55
1:A:870:ILE:HA	1:A:873:LEU:HD12	1.89	0.55
1:A:834:LYS:HG3	1:A:903:MET:SD	2.46	0.55
1:A:23:LYS:O	1:A:27:GLU:HG2	2.08	0.54
1:A:424:LEU:HB2	1:A:425:PRO:HD3	1.88	0.54
1:A:86:PHE:HB3	1:A:198:LYS:O	2.06	0.54
1:A:939:TYR:CE1	1:A:1044:ALA:HB2	2.42	0.54
1:A:583:LEU:HD12	1:A:584:PRO:HD2	1.89	0.54
1:A:441:SER:HB2	1:A:467:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PHE:HD2	1:A:88:PHE:HE1	1.54	0.54
1:A:289:LEU:HD23	1:A:325:ILE:HB	1.89	0.54
1:A:420:ASP:N	1:A:420:ASP:OD1	2.41	0.54
1:A:48:VAL:HG12	1:A:670:LEU:HB3	1.88	0.54
1:A:95:MET:H	1:A:96:PRO:HD3	1.72	0.54
1:A:870:ILE:O	1:A:873:LEU:HB2	2.07	0.54
1:A:481:GLY:C	1:A:483:LYS:HE2	2.29	0.53
1:A:162:LYS:HD2	1:A:166:LEU:O	2.08	0.53
1:A:45:LYS:HE2	1:A:669:ASP:OD2	2.09	0.53
1:A:106:ARG:NH2	5:A:1203:HOH:O	2.15	0.53
1:A:255:THR:HB	1:A:515:MET:H	1.73	0.53
1:A:564:THR:HG21	1:A:679:PRO:HA	1.89	0.53
1:A:350:LYS:HE2	5:A:1236:HOH:O	2.07	0.53
1:A:949:HIS:NE2	1:A:1010:LEU:HD22	2.23	0.53
1:A:543:THR:HG21	1:A:687:TYR:CD1	2.44	0.52
1:A:266:LEU:HB3	1:A:505:LEU:O	2.10	0.52
1:A:685:TYR:OH	1:A:701:PRO:HB3	2.09	0.52
1:A:705:ARG:HH22	1:A:748:ASP:HA	1.75	0.52
1:A:220:TRP:CH2	1:A:639:PHE:HD2	2.28	0.52
1:A:795:ARG:HB3	1:A:895:LEU:HD11	1.91	0.52
1:A:92:CYS:O	1:A:94:GLY:N	2.35	0.52
1:A:568:LEU:HD23	1:A:687:TYR:CE2	2.44	0.52
1:A:459:LYS:H	1:A:459:LYS:HD2	1.74	0.52
1:A:909:LEU:HD21	1:A:1059:ASN:OD1	2.10	0.52
1:A:955:LEU:HD22	1:A:966:LEU:CD2	2.40	0.52
1:A:282:LEU:CD2	1:A:285:LYS:HE3	2.40	0.51
1:A:976:LEU:HD13	1:A:989:VAL:HG13	1.93	0.51
1:A:543:THR:HG22	1:A:690:VAL:CB	2.40	0.51
1:A:345:VAL:O	1:A:347:PRO:HD3	2.10	0.51
1:A:463:ALA:O	1:A:467:ILE:HG22	2.11	0.51
1:A:87:PRO:HB2	1:A:604:TYR:CD1	2.46	0.51
1:A:608:HIS:CE1	1:A:609:LEU:HG	2.45	0.51
1:A:873:LEU:C	1:A:875:GLY:H	2.15	0.51
1:A:200:ASP:OD2	1:A:202:ARG:NH2	2.38	0.50
1:A:543:THR:HG22	1:A:690:VAL:HB	1.94	0.50
1:A:623:LEU:HD22	1:A:654:LYS:HD2	1.93	0.50
1:A:949:HIS:CD2	1:A:1010:LEU:HD22	2.46	0.50
1:A:95:MET:H	1:A:96:PRO:CD	2.25	0.50
1:A:404:ARG:HH21	1:A:443:VAL:CG2	2.24	0.50
1:A:836:ARG:HA	1:A:843:MET:SD	2.52	0.50
1:A:1024:ILE:HA	1:A:1027:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:PHE:HE1	1:A:470:LYS:HD3	1.76	0.50
1:A:539:TRP:O	1:A:543:THR:HG23	2.12	0.49
1:A:712:LEU:O	1:A:715:GLU:HB2	2.11	0.49
1:A:307:VAL:HG12	1:A:388:VAL:HG22	1.93	0.49
1:A:690:VAL:O	1:A:694:PRO:HA	2.12	0.49
1:A:432:ILE:HD12	1:A:487:VAL:HG11	1.94	0.49
1:A:773:TRP:O	1:A:777:MET:HG2	2.12	0.49
1:A:58:ARG:NE	1:A:187:LEU:HD13	2.28	0.49
1:A:1044:ALA:N	5:A:1212:HOH:O	2.46	0.49
1:A:1049:ARG:O	1:A:1049:ARG:HG2	2.12	0.49
1:A:92:CYS:HB2	1:A:208:THR:CG2	2.41	0.49
1:A:292:ALA:HB2	1:A:386:THR:HG23	1.95	0.49
1:A:892:ASN:O	1:A:896:ILE:HG13	2.12	0.49
1:A:529:GLN:OE1	1:A:572:ALA:HB2	2.13	0.49
1:A:621:SER:OG	1:A:624:GLY:N	2.46	0.49
1:A:939:TYR:CD2	1:A:1048:ILE:HG21	2.48	0.48
1:A:58:ARG:CZ	1:A:187:LEU:HD13	2.44	0.48
1:A:614:ASN:HD22	1:A:619:ALA:HB2	1.78	0.48
1:A:242:PRO:HB3	1:A:336:TYR:OH	2.13	0.48
1:A:828:PHE:HE2	1:A:854:VAL:HG12	1.78	0.48
1:A:885:TRP:CD2	1:A:886:PRO:HD2	2.48	0.48
1:A:601:MET:HE2	1:A:671:ARG:HD2	1.95	0.48
1:A:92:CYS:SG	1:A:206:ILE:HG23	2.54	0.48
1:A:270:LYS:HE3	5:A:1205:HOH:O	2.14	0.48
1:A:440:LEU:HB3	1:A:443:VAL:HG12	1.94	0.48
1:A:480:ASP:HA	1:A:483:LYS:CG	2.43	0.48
1:A:433:GLU:HB2	1:A:478:LEU:HD11	1.95	0.48
1:A:185:PRO:HB2	1:A:186:PRO:HD3	1.95	0.48
1:A:308:ARG:HG2	1:A:310:ASP:OD1	2.13	0.48
1:A:208:THR:HG21	1:A:579:LEU:HD13	1.95	0.47
1:A:947:TRP:O	1:A:951:THR:HG23	2.14	0.47
1:A:202:ARG:HE	1:A:202:ARG:HB2	1.52	0.47
1:A:237:TYR:O	1:A:238:THR:HG23	2.13	0.47
1:A:599:ILE:HD13	1:A:692:MET:HG3	1.95	0.47
1:A:278:LYS:CE	1:A:350:LYS:HE3	2.44	0.47
1:A:911:LEU:O	1:A:913:LEU:N	2.48	0.47
1:A:158:TRP:CZ3	1:A:171:ILE:HB	2.49	0.47
1:A:308:ARG:NH1	1:A:380:ILE:H	2.12	0.47
1:A:319:VAL:HG23	1:A:341:LYS:HA	1.97	0.47
1:A:58:ARG:HD3	1:A:187:LEU:HD13	1.96	0.47
1:A:308:ARG:NH1	1:A:380:ILE:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:CYS:O	1:A:1036:ILE:HA	2.14	0.47
1:A:252:ASP:OD2	1:A:575:ARG:NH1	2.34	0.47
1:A:461:ALA:O	1:A:465:GLU:HG3	2.15	0.47
1:A:28:ARG:NE	5:A:1209:HOH:O	2.42	0.47
1:A:719:LYS:N	2:A:1102:PO4:O3	2.45	0.47
1:A:735:SER:O	1:A:739:MET:N	2.42	0.47
1:A:376:PRO:HD2	1:A:406:LEU:HD11	1.96	0.47
1:A:477:MET:HG2	1:A:487:VAL:HG12	1.96	0.47
1:A:275:TYR:CZ	1:A:287:ILE:HD12	2.50	0.47
1:A:404:ARG:NH2	5:A:1211:HOH:O	2.45	0.46
1:A:955:LEU:HD22	1:A:966:LEU:HD21	1.96	0.46
1:A:43:LYS:HD3	1:A:82:LYS:HG2	1.96	0.46
1:A:77:GLN:HG3	1:A:82:LYS:HG3	1.98	0.46
1:A:1043:GLU:O	1:A:1043:GLU:HG2	2.14	0.46
1:A:760:ALA:O	1:A:764:ILE:HG13	2.16	0.46
1:A:726:THR:OG1	1:A:729:GLN:HG3	2.16	0.46
1:A:911:LEU:C	1:A:913:LEU:H	2.19	0.46
1:A:300:PHE:HB2	1:A:431:VAL:HG21	1.96	0.46
1:A:605:THR:O	1:A:661:GLU:HG2	2.16	0.46
1:A:52:TYR:CD1	1:A:600:TYR:CE2	3.04	0.46
1:A:330:ALA:O	1:A:334:MET:HG3	2.15	0.46
1:A:278:LYS:HG3	1:A:278:LYS:O	2.16	0.45
1:A:378:LEU:N	1:A:378:LEU:HD22	2.31	0.45
1:A:543:THR:HG22	1:A:690:VAL:HG21	1.98	0.45
1:A:696:GLN:NE2	1:A:699:LYS:HG3	2.30	0.45
1:A:784:LEU:HD13	1:A:845:ARG:HA	1.99	0.45
1:A:92:CYS:SG	1:A:206:ILE:HD12	2.56	0.45
1:A:909:LEU:HD23	1:A:909:LEU:HA	1.81	0.45
1:A:43:LYS:HE2	1:A:43:LYS:HB3	1.57	0.45
1:A:575:ARG:NH2	1:A:592:GLU:OE1	2.50	0.45
1:A:940:VAL:N	1:A:1041:ALA:HB2	2.32	0.45
1:A:43:LYS:CG	1:A:82:LYS:HG2	2.44	0.45
1:A:75:GLY:HA2	1:A:198:LYS:HE2	1.97	0.45
1:A:464:LYS:O	1:A:468:TYR:HB2	2.16	0.45
1:A:692:MET:O	1:A:694:PRO:HD3	2.17	0.45
1:A:895:LEU:O	1:A:898:SER:OG	2.25	0.45
1:A:406:LEU:HD23	1:A:412:LEU:HB3	1.99	0.45
1:A:565:LEU:HA	1:A:565:LEU:HD23	1.62	0.45
1:A:90:LEU:HB2	1:A:206:ILE:HD13	1.98	0.45
1:A:51:PRO:HA	1:A:671:ARG:HH22	1.82	0.45
1:A:208:THR:HB	1:A:579:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:HIS:N	1:A:752:ASP:OD1	2.44	0.45
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.70	0.44
1:A:180:TRP:CD1	1:A:180:TRP:N	2.85	0.44
1:A:748:ASP:OD1	1:A:748:ASP:N	2.49	0.44
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.79	0.44
1:A:629:GLN:NE2	1:A:649:GLN:HB2	2.32	0.44
1:A:789:ALA:HB2	1:A:844:HIS:CD2	2.52	0.44
1:A:381:LYS:HB3	1:A:383:ASP:OD1	2.16	0.44
1:A:972:ILE:HD13	1:A:993:VAL:HG11	1.99	0.44
1:A:52:TYR:HD1	1:A:52:TYR:H	1.65	0.44
1:A:54:TYR:N	3:A:1104:LSS:HN2	2.16	0.44
1:A:214:TYR:O	1:A:218:VAL:HG23	2.17	0.44
1:A:215:ASP:OD2	1:A:581:THR:HG23	2.18	0.44
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.75	0.44
1:A:782:ASP:C	1:A:784:LEU:H	2.21	0.44
1:A:789:ALA:HB2	1:A:844:HIS:CE1	2.52	0.44
1:A:1035:HIS:C	1:A:1036:ILE:HG13	2.37	0.44
1:A:34:ALA:HB2	1:A:665:TRP:NE1	2.33	0.44
1:A:45:LYS:O	1:A:45:LYS:HG3	2.17	0.44
1:A:266:LEU:CD1	1:A:290:VAL:HG22	2.47	0.44
1:A:480:ASP:HA	1:A:483:LYS:HG3	1.99	0.44
1:A:531:TYR:CD1	1:A:570:GLU:HB3	2.53	0.44
1:A:532:LEU:HD23	1:A:532:LEU:HA	1.65	0.44
1:A:304:ASN:ND2	1:A:375:LEU:HD12	2.33	0.43
1:A:92:CYS:O	1:A:97:ILE:HD13	2.18	0.43
1:A:20:ILE:HD13	1:A:20:ILE:HA	1.78	0.43
1:A:262:GLN:HB2	1:A:511:GLU:CG	2.47	0.43
1:A:378:LEU:HD22	1:A:378:LEU:H	1.83	0.43
1:A:913:LEU:HD22	1:A:1031:LEU:HD12	2.00	0.43
1:A:1017:LYS:NZ	1:A:1038:VAL:O	2.40	0.43
1:A:379:THR:O	1:A:379:THR:OG1	2.29	0.43
1:A:995:MET:O	1:A:998:GLU:HB2	2.18	0.43
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.34	0.43
1:A:376:PRO:HD3	1:A:418:ILE:CD1	2.46	0.43
1:A:48:VAL:O	1:A:87:PRO:HD2	2.19	0.43
1:A:282:LEU:HD22	1:A:285:LYS:HE3	2.00	0.43
1:A:530:TRP:HB2	1:A:574:SER:HB3	2.01	0.43
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.81	0.43
1:A:80:LYS:HD2	1:A:80:LYS:HA	1.65	0.43
1:A:486:LYS:HG3	1:A:489:ASP:OD2	2.18	0.43
1:A:936:CYS:SG	1:A:1036:ILE:HG23	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:ILE:HG21	1:A:993:VAL:HG11	2.01	0.43
1:A:48:VAL:HG23	1:A:86:PHE:CD1	2.54	0.43
1:A:101:ALA:HB1	1:A:175:SER:O	2.19	0.42
1:A:686:LEU:CD2	1:A:701:PRO:HG2	2.49	0.42
1:A:976:LEU:HD13	1:A:989:VAL:CG1	2.49	0.42
1:A:48:VAL:HG21	1:A:70:CYS:HB2	2.01	0.42
1:A:58:ARG:CD	1:A:187:LEU:HD13	2.49	0.42
1:A:232:LYS:HB2	1:A:531:TYR:CE2	2.54	0.42
1:A:254:GLN:HA	1:A:254:GLN:OE1	2.19	0.42
1:A:282:LEU:HD11	1:A:349:VAL:CG2	2.49	0.42
1:A:866:LEU:HD23	1:A:866:LEU:HA	1.60	0.42
1:A:899:SER:O	1:A:903:MET:HG3	2.19	0.42
1:A:270:LYS:HA	1:A:288:PHE:CD1	2.54	0.42
1:A:955:LEU:HD13	1:A:996:ILE:HG21	2.01	0.42
1:A:276:PRO:HD2	1:A:279:LEU:HD12	2.01	0.42
1:A:909:LEU:HD11	1:A:1059:ASN:ND2	2.35	0.42
1:A:611:GLN:NE2	1:A:614:ASN:O	2.53	0.42
1:A:796:VAL:HG21	1:A:899:SER:HB3	2.02	0.42
1:A:892:ASN:HB3	1:A:895:LEU:HB2	2.02	0.42
1:A:1040:PHE:HB2	5:A:1248:HOH:O	2.19	0.42
1:A:55:MET:HE2	1:A:184:PHE:HB3	2.00	0.42
1:A:93:THR:HG21	1:A:596:ASP:OD2	2.20	0.42
1:A:445:ILE:HA	1:A:448:GLU:HG2	2.01	0.42
1:A:54:TYR:H	3:A:1104:LSS:HN2	1.67	0.42
1:A:60:HIS:O	1:A:64:THR:HG23	2.20	0.42
1:A:220:TRP:CZ3	1:A:639:PHE:HD2	2.38	0.42
1:A:37:LEU:HD13	1:A:83:CYS:CB	2.50	0.42
1:A:226:ARG:HB2	1:A:585:TRP:CH2	2.55	0.42
1:A:601:MET:HE3	1:A:671:ARG:CZ	2.50	0.42
1:A:1033:LEU:HB3	1:A:1034:GLU:H	1.72	0.42
1:A:72:PHE:HB2	1:A:817:PHE:CE2	2.54	0.41
1:A:93:THR:HG23	1:A:580:GLY:HA2	2.02	0.41
1:A:179:HIS:O	1:A:182:ASP:HB2	2.20	0.41
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.86	0.41
1:A:65:PHE:CB	1:A:710:LEU:HD13	2.50	0.41
1:A:266:LEU:HD12	1:A:291:ALA:O	2.20	0.41
1:A:71:GLU:OE2	1:A:740:ARG:NH2	2.48	0.41
1:A:38:GLU:O	1:A:38:GLU:HG2	2.20	0.41
1:A:893:GLU:O	1:A:896:ILE:N	2.53	0.41
1:A:45:LYS:HZ1	1:A:667:PRO:HD2	1.85	0.41
1:A:93:THR:HG23	1:A:580:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HB2	1:A:157:GLN:HG2	2.02	0.41
1:A:646:PRO:O	1:A:648:THR:N	2.51	0.41
1:A:1031:LEU:HD13	1:A:1031:LEU:HA	1.84	0.41
1:A:282:LEU:HD23	1:A:285:LYS:HE3	2.03	0.41
1:A:634:VAL:O	1:A:638:VAL:HG23	2.20	0.41
1:A:696:GLN:HE22	1:A:699:LYS:HE2	1.86	0.41
1:A:63:HIS:CD2	3:A:1104:LSS:H25	2.56	0.41
1:A:79:LEU:C	1:A:81:GLY:N	2.75	0.41
1:A:206:ILE:CG2	1:A:207:THR:N	2.84	0.41
1:A:686:LEU:O	1:A:687:TYR:C	2.60	0.41
1:A:913:LEU:C	1:A:915:ASN:H	2.25	0.40
1:A:52:TYR:CE2	1:A:91:HIS:CD2	3.09	0.40
1:A:306:TRP:CE3	1:A:377:MET:HB2	2.56	0.40
1:A:623:LEU:HD13	1:A:654:LYS:HB3	2.02	0.40
1:A:252:ASP:C	1:A:517:ARG:HG2	2.41	0.40
1:A:323:ILE:HD12	1:A:349:VAL:HG11	2.02	0.40
1:A:376:PRO:HD2	1:A:406:LEU:CD1	2.51	0.40
1:A:915:ASN:HB2	1:A:916:TYR:CD1	2.55	0.40
1:A:950:THR:O	1:A:954:VAL:HG23	2.20	0.40
1:A:253:ARG:HD3	1:A:514:VAL:CG1	2.51	0.40
1:A:470:LYS:HE3	1:A:474:GLU:OE1	2.22	0.40
1:A:1027:LEU:HD23	1:A:1027:LEU:HA	1.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	998/1073 (93%)	875 (88%)	107 (11%)	16 (2%)	9 40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	SER
1	A	304	ASN
1	A	456	ASP
1	A	483	LYS
1	A	511	GLU
1	A	696	GLN
1	A	874	LEU
1	A	1012	LEU
1	A	93	THR
1	A	652	LYS
1	A	781	TRP
1	A	981	GLU
1	A	912	ARG
1	A	465	GLU
1	A	587	GLU
1	A	51	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	885/941 (94%)	857 (97%)	28 (3%)	39 70

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	43	LYS
1	A	70	CYS
1	A	95	MET
1	A	283	LYS
1	A	329	LYS
1	A	352	LEU
1	A	398	ASP
1	A	420	ASP
1	A	558	ARG
1	A	559	ARG

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Mol	Chain	Res	Type
1	A	604	TYR
1	A	608	HIS
1	A	621	SER
1	A	652	LYS
1	A	666	TYR
1	A	688	ASN
1	A	707	ASN
1	A	734	PHE
1	A	759	MET
1	A	828	PHE
1	A	834	LYS
1	A	866	LEU
1	A	899	SER
1	A	935	HIS
1	A	1006	ARG
1	A	1040	PHE
1	A	1042	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	A	696	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

5 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	PO4	A	1101	-	4,4,4	2.44	2 (50%)	6,6,6	1.34	1 (16%)
2	PO4	A	1102	-	4,4,4	3.68	3 (75%)	6,6,6	2.51	4 (66%)
3	LSS	A	1104	1	30,33,33	6.34	13 (43%)	33,49,49	4.10	12 (36%)
2	PO4	A	1103	-	4,4,4	2.96	4 (100%)	6,6,6	0.43	0
4	LEU	A	1105	-	7,8,8	0.82	0	9,10,10	1.28	2 (22%)

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
4	LEU	A	1105	-	-	2/8/8/8	-
3	LSS	A	1104	1	-	11/18/39/39	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1104	LSS	O2A-S1	28.46	1.66	1.42
3	A	1104	LSS	C23-C22	-10.55	1.24	1.53
3	A	1104	LSS	C22-C21	7.51	1.65	1.53
3	A	1104	LSS	O4-C21	-6.86	1.31	1.41
3	A	1104	LSS	S1-N2	6.42	1.71	1.59
3	A	1104	LSS	O1A-S1	5.84	1.47	1.42
2	A	1102	PO4	P-O1	5.74	1.64	1.50
3	A	1104	LSS	C1-N2	5.64	1.48	1.37
2	A	1103	PO4	P-O1	4.52	1.61	1.50
3	A	1104	LSS	O5-S1	4.15	1.68	1.59
2	A	1101	PO4	P-O1	3.99	1.60	1.50
3	A	1104	LSS	C6-N6	3.62	1.47	1.34
2	A	1102	PO4	P-O4	3.37	1.64	1.54
3	A	1104	LSS	C25-C24	-3.23	1.41	1.51
3	A	1104	LSS	O3-C23	2.97	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1104	LSS	C23-C24	2.58	1.59	1.53
2	A	1102	PO4	P-O2	2.42	1.61	1.54
3	A	1104	LSS	O4-C24	2.32	1.50	1.45
2	A	1103	PO4	P-O3	2.29	1.61	1.54
2	A	1103	PO4	P-O2	2.26	1.61	1.54
2	A	1101	PO4	P-O4	2.06	1.60	1.54
2	A	1103	PO4	P-O4	-2.05	1.48	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1104	LSS	O2A-S1-O1A	-13.75	99.34	120.76
3	A	1104	LSS	O5-S1-O2A	13.33	146.34	105.59
3	A	1104	LSS	C1-N2-S1	-7.53	112.42	124.61
3	A	1104	LSS	O5-S1-N2	-4.78	92.26	105.60
3	A	1104	LSS	C23-C22-C21	4.65	107.97	100.98
3	A	1104	LSS	N3-C2-N1	-4.34	121.90	128.68
2	A	1102	PO4	O2-P-O1	-3.81	96.95	110.89
3	A	1104	LSS	O1-C1-N2	-3.40	116.46	123.00
2	A	1102	PO4	O4-P-O2	3.34	118.69	107.97
3	A	1104	LSS	C4-C5-N7	-3.33	105.93	109.40
3	A	1104	LSS	C9-CA-C1	-3.20	103.92	110.85
3	A	1104	LSS	O5-S1-O1A	-3.13	96.02	105.59
3	A	1104	LSS	C22-C23-C24	2.64	107.77	102.64
2	A	1102	PO4	O4-P-O3	-2.62	99.55	107.97
4	A	1105	LEU	OXT-C-O	-2.58	118.24	124.09
4	A	1105	LEU	OXT-C-CA	2.38	121.50	113.38
2	A	1101	PO4	O4-P-O2	2.23	115.12	107.97
3	A	1104	LSS	O3-C23-C24	-2.16	104.80	111.05
2	A	1102	PO4	O4-P-O1	2.05	118.39	110.89

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1104	LSS	O1-C1-CA-C9
3	A	1104	LSS	C1-N2-S1-O2A
3	A	1104	LSS	C23-C24-C25-O5
3	A	1104	LSS	O4-C24-C25-O5
3	A	1104	LSS	C11-C7-C9-CA
4	A	1105	LEU	C-CA-CB-CG
3	A	1104	LSS	C10-C7-C9-CA

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Mol	Chain	Res	Type	Atoms
3	A	1104	LSS	C25-O5-S1-O1A
3	A	1104	LSS	C25-O5-S1-O2A
3	A	1104	LSS	O1-C1-CA-N4
3	A	1104	LSS	N2-C1-CA-N4
3	A	1104	LSS	N2-C1-CA-C9
4	A	1105	LEU	N-CA-CB-CG

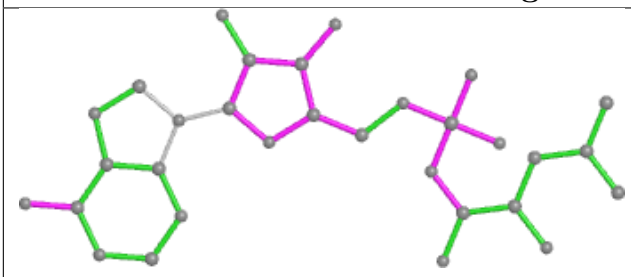
There are no ring outliers.

2 monomers are involved in 7 short contacts:

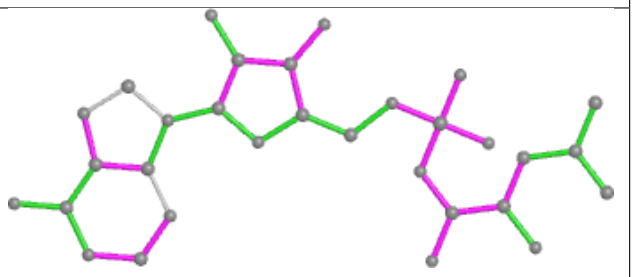
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	PO4	1	0
3	A	1104	LSS	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

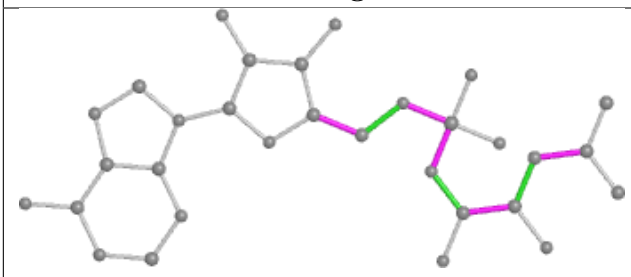
Ligand LSS A 1104



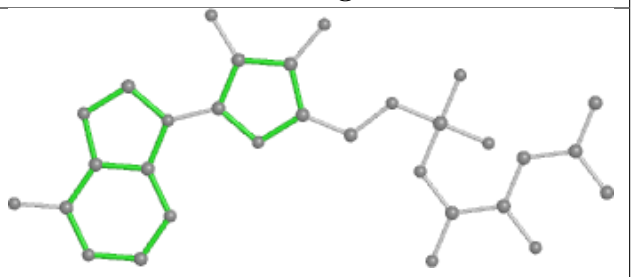
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.

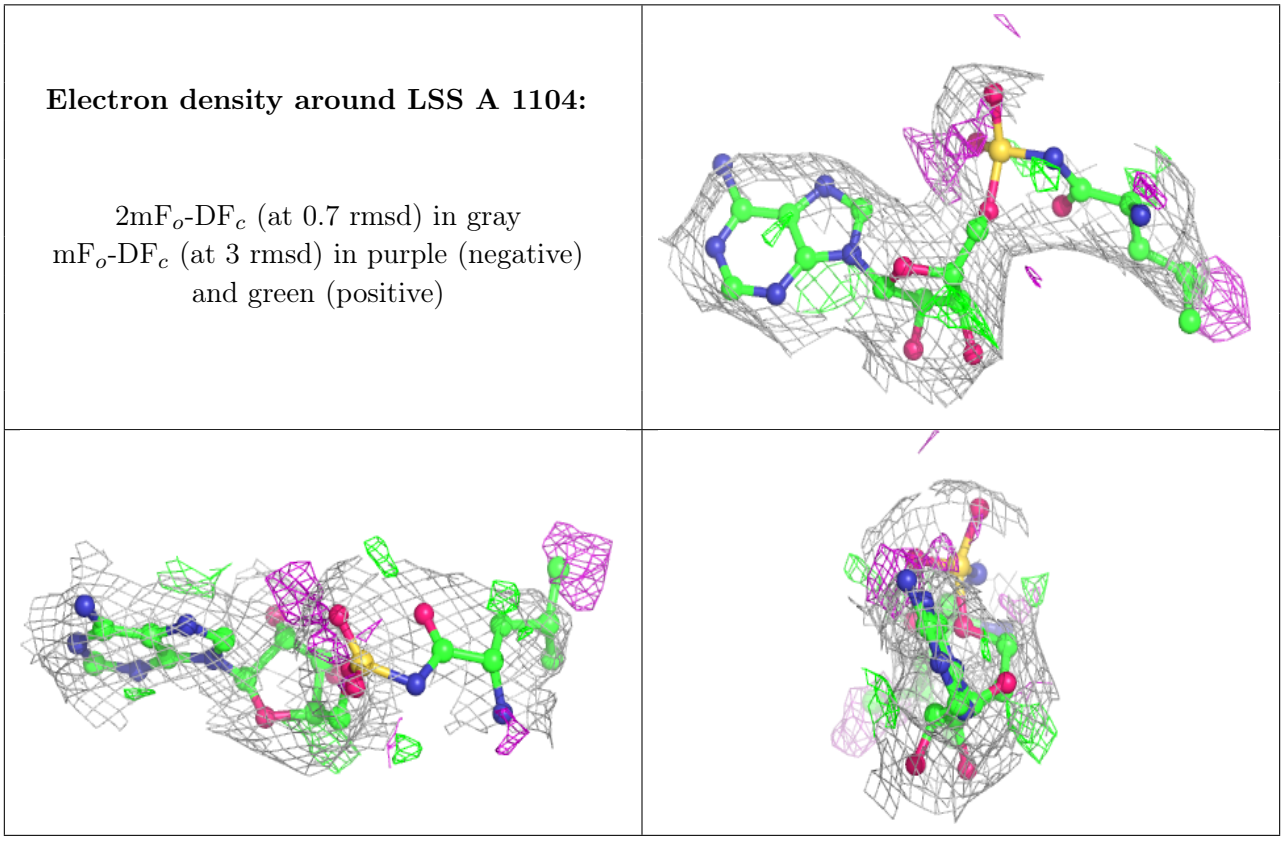
6.4 Ligands

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 LSS A 1104:

$2mF_o$-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.