



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:55 AM UTC

PDB ID : 8HLK / pdb_00008hbk
Title : Structure of McyB-C1A1 complexed with L-Leu and AMP
Authors : Peng, Y.J.
Deposited on : 2022-11-30
Resolution : 2.70 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

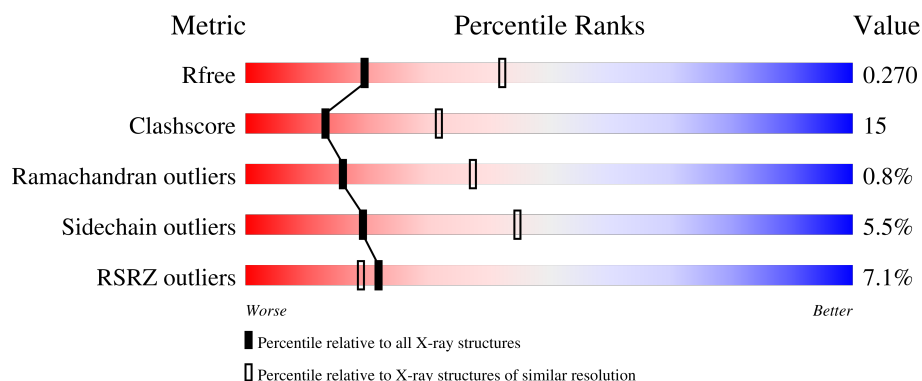
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	967	

2 Entry composition [i](#)

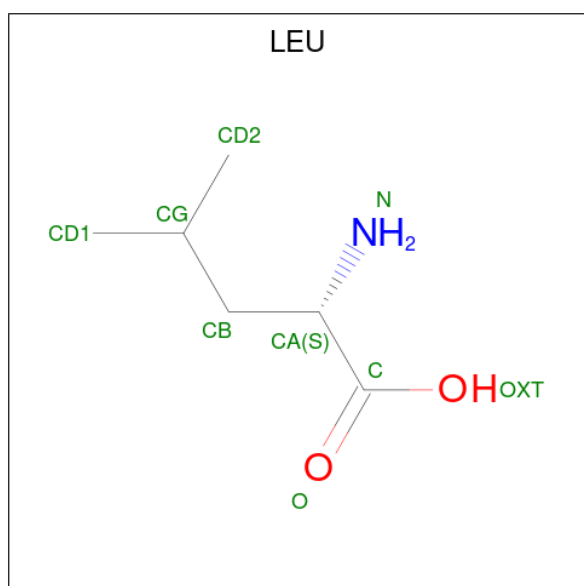
There are 4 unique types of molecules in this entry. The entry contains 7536 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Microcystin synthetase B (Fragment).

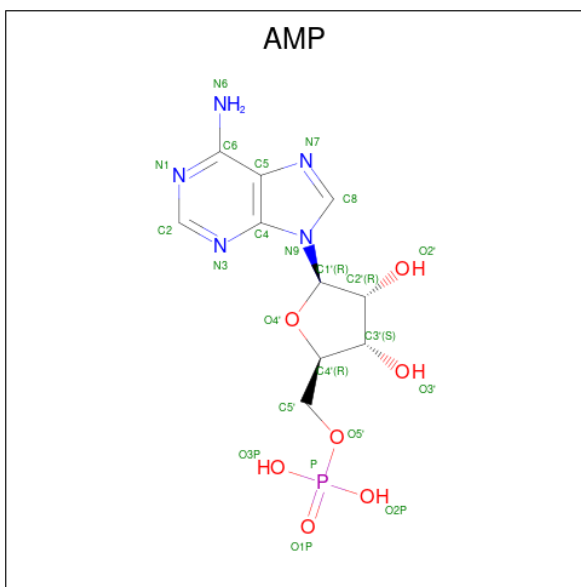
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	910	7301	4686	1231	1363	21	0	0	0

- Molecule 2 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

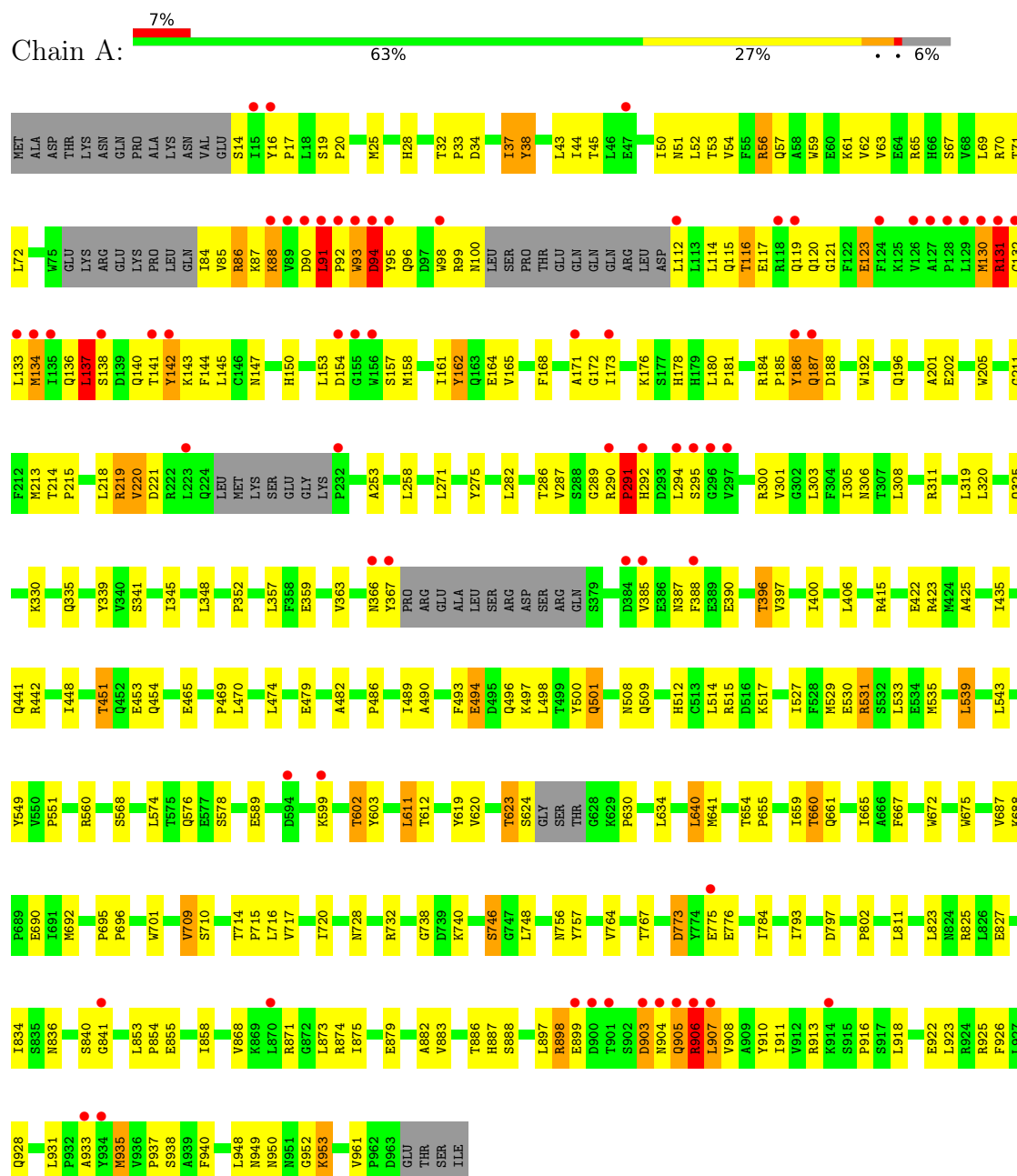
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Microcystin synthetase B (Fragment)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.53Å 152.53Å 135.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	13.15 – 2.70 13.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (13.15-2.70) 98.9 (13.15-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.213 , 0.269 0.221 , 0.270	Depositor DCC
R_{free} test set	2540 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7536	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.66	0/7469	1.26	33/10166 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ILE	N-CA-C	-19.22	93.81	112.83
1	A	220	VAL	N-CA-C	-12.30	101.17	113.10
1	A	186	TYR	CB-CA-C	-11.78	92.03	111.23
1	A	187	GLN	N-CA-C	-7.98	103.12	113.17
1	A	219	ARG	CB-CA-C	-7.91	94.68	110.42
1	A	953	LYS	CB-CA-C	-7.65	97.38	109.70
1	A	907	LEU	N-CA-C	7.43	121.64	110.64
1	A	903	ASP	N-CA-C	7.37	120.74	111.24
1	A	137	LEU	CB-CA-C	6.87	120.79	109.72
1	A	71	THR	CA-CB-OG1	-6.87	99.30	109.60
1	A	938	SER	N-CA-C	6.83	118.72	111.28
1	A	938	SER	CB-CA-C	-6.44	100.09	110.79
1	A	286	THR	CA-CB-OG1	-6.43	99.95	109.60
1	A	352	PRO	N-CA-CB	6.20	106.66	103.19
1	A	441	GLN	N-CA-CB	-6.04	101.47	110.17
1	A	515	ARG	CB-CA-C	5.95	121.80	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	THR	CA-CB-OG1	-5.86	100.81	109.60
1	A	879	GLU	CB-CG-CD	5.85	122.55	112.60
1	A	797	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	291	PRO	N-CA-CB	-5.79	97.17	103.25
1	A	660	THR	CB-CA-C	5.75	119.33	109.51
1	A	94	ASP	CB-CA-C	-5.70	99.12	109.38
1	A	116	THR	N-CA-C	-5.51	104.30	111.02
1	A	479	GLU	CB-CA-C	5.49	120.69	109.55
1	A	623	THR	CB-CA-C	-5.46	100.27	109.83
1	A	903	ASP	CB-CA-C	-5.45	101.86	110.86
1	A	38	TYR	N-CA-CB	-5.39	102.51	110.49
1	A	95	TYR	N-CA-C	5.35	117.97	109.24
1	A	308	LEU	O-C-N	-5.32	118.10	121.88
1	A	162	TYR	N-CA-CB	5.24	117.61	110.01
1	A	465	GLU	CB-CG-CD	5.12	121.31	112.60
1	A	667	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	95	TYR	N-CA-CB	-5.05	102.20	110.43

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	GLY	Peptide
1	A	131	ARG	Sidechain
1	A	423	ARG	Sidechain
1	A	531	ARG	Sidechain
1	A	56	ARG	Sidechain
1	A	825	ARG	Sidechain
1	A	86	ARG	Sidechain
1	A	906	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7301	0	7307	219	0
2	A	9	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	12	1	0
4	A	203	0	0	11	0
All	All	7536	0	7329	219	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 15.

All (219) 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:120:GLN:O	1:A:123:GLU:OE2	1.65	1.09
1:A:836:ASN:CB	1:A:841:GLY:O	2.13	0.95
1:A:300:ARG:HD3	4:A:1415:HOH:O	1.66	0.94
1:A:496:GLN:HB3	1:A:533:LEU:HD11	1.52	0.89
1:A:531:ARG:HD2	1:A:661:GLN:OE1	1.72	0.89
1:A:836:ASN:HB2	1:A:841:GLY:O	1.73	0.88
1:A:96:GLN:NE2	1:A:98:TRP:O	2.08	0.87
1:A:186:TYR:O	1:A:186:TYR:CG	2.25	0.86
1:A:186:TYR:O	1:A:186:TYR:CD2	2.31	0.84
1:A:836:ASN:HB3	1:A:841:GLY:O	1.78	0.84
1:A:918:LEU:HD21	1:A:923:LEU:HD13	1.60	0.82
1:A:357:LEU:HD23	1:A:357:LEU:H	1.46	0.80
1:A:489:ILE:HD12	1:A:497:LYS:HD3	1.62	0.80
1:A:221:ASP:O	4:A:1301:HOH:O	2.01	0.79
1:A:931:LEU:HD23	1:A:935:MET:HB3	1.66	0.77
1:A:793:ILE:HD11	1:A:858:ILE:HD11	1.69	0.73
1:A:320:LEU:HD21	1:A:435:ILE:HG12	1.71	0.72
1:A:738:GLY:HA2	2:A:1201:LEU:N	2.06	0.71
1:A:923:LEU:HD23	1:A:940:PHE:CD2	2.26	0.71
1:A:150:HIS:O	1:A:303:LEU:HD13	1.92	0.70
1:A:907:LEU:O	1:A:907:LEU:HG	1.92	0.69
1:A:98:TRP:HE3	1:A:99:ARG:O	1.75	0.68
1:A:16:TYR:CE2	1:A:187:GLN:HB3	2.28	0.68
1:A:214:THR:OG1	1:A:215:PRO:HD2	1.93	0.68
1:A:59:TRP:O	1:A:62:VAL:HG22	1.94	0.68
1:A:115:GLN:HA	1:A:119:GLN:HB2	1.76	0.67
1:A:115:GLN:HG3	1:A:116:THR:H	1.60	0.67
1:A:527:ILE:HG13	1:A:529:MET:HE2	1.75	0.66
1:A:923:LEU:HD23	1:A:940:PHE:HD2	1.61	0.65
1:A:72:LEU:CD2	1:A:87:LYS:HB2	2.27	0.65
1:A:486:PRO:HB3	1:A:501:GLN:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:O	1:A:120:GLN:N	2.30	0.64
1:A:531:ARG:CD	1:A:661:GLN:OE1	2.44	0.64
1:A:660:THR:HG22	1:A:710:SER:HA	1.78	0.64
1:A:43:LEU:HD13	1:A:145:LEU:HD12	1.78	0.64
1:A:469:PRO:HG2	1:A:641:MET:CE	2.27	0.63
1:A:271:LEU:CD1	1:A:448:ILE:HD11	2.28	0.63
1:A:474:LEU:HD23	1:A:543:LEU:HD21	1.81	0.63
1:A:623:THR:O	1:A:630:PRO:HB3	2.00	0.62
1:A:773:ASP:OD1	1:A:773:ASP:N	2.25	0.62
1:A:67:SER:HB2	1:A:88:LYS:HG3	1.84	0.60
1:A:202:GLU:HA	1:A:348:LEU:HD21	1.84	0.60
1:A:341:SER:O	1:A:345:ILE:HG13	2.01	0.59
1:A:740:LYS:HE2	4:A:1444:HOH:O	2.02	0.59
1:A:517:LYS:NZ	1:A:589:GLU:OE2	2.36	0.58
1:A:933:ALA:C	1:A:935:MET:H	2.08	0.58
1:A:63:VAL:HG11	1:A:93:TRP:HA	1.86	0.58
1:A:45:THR:HG22	1:A:143:LYS:HD3	1.86	0.58
1:A:56:ARG:NH1	1:A:96:GLN:HB2	2.18	0.58
1:A:767:THR:HG22	1:A:784:ILE:O	2.04	0.58
1:A:72:LEU:HB3	1:A:130:MET:HA	1.85	0.57
1:A:157:SER:HB3	1:A:301:VAL:HG13	1.87	0.57
1:A:898:ARG:HB2	1:A:905:GLN:HA	1.87	0.57
1:A:827:GLU:HG2	4:A:1323:HOH:O	2.05	0.56
1:A:28:HIS:O	1:A:32:THR:OG1	2.17	0.56
1:A:490:ALA:HB2	1:A:500:TYR:CD1	2.40	0.56
1:A:688:LYS:HB3	1:A:690:GLU:HG2	1.87	0.56
1:A:205:TRP:CE2	1:A:345:ILE:HD13	2.41	0.56
1:A:120:GLN:HE22	1:A:387:ASN:HD22	1.54	0.56
1:A:660:THR:HG21	1:A:710:SER:OG	2.04	0.56
1:A:287:VAL:HG21	1:A:335:GLN:HG2	1.86	0.56
1:A:937:PRO:HD2	1:A:940:PHE:CZ	2.41	0.56
1:A:98:TRP:H	1:A:137:LEU:HD12	1.71	0.55
1:A:469:PRO:HG2	1:A:641:MET:HE2	1.87	0.55
1:A:887:HIS:ND1	1:A:888:SER:O	2.40	0.55
1:A:94:ASP:OD2	1:A:94:ASP:N	2.40	0.55
1:A:16:TYR:CD2	1:A:187:GLN:HB3	2.42	0.55
1:A:568:SER:HA	1:A:823:LEU:HD21	1.88	0.55
1:A:171:ALA:HB3	1:A:178:HIS:HB2	1.88	0.54
1:A:899:GLU:HG3	1:A:961:VAL:HG22	1.89	0.54
1:A:660:THR:HG23	4:A:1320:HOH:O	2.07	0.54
1:A:287:VAL:HG23	1:A:335:GLN:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:GLN:HE21	1:A:578:SER:HB3	1.73	0.54
1:A:86:ARG:CZ	1:A:86:ARG:HB3	2.36	0.54
1:A:659:ILE:HG12	1:A:709:VAL:HG13	1.90	0.54
1:A:201:ALA:HB2	1:A:339:TYR:CE1	2.43	0.53
1:A:178:HIS:NE2	1:A:180:LEU:HD11	2.24	0.53
1:A:53:THR:O	1:A:57:GLN:HG3	2.09	0.53
1:A:907:LEU:O	1:A:937:PRO:HB3	2.09	0.53
1:A:154:ASP:HB3	1:A:306:ASN:HD21	1.74	0.53
1:A:732:ARG:NH1	4:A:1311:HOH:O	2.36	0.53
1:A:72:LEU:HD21	1:A:87:LYS:HB2	1.90	0.52
1:A:72:LEU:HD23	1:A:87:LYS:O	2.10	0.52
1:A:271:LEU:HD12	1:A:448:ILE:HD11	1.91	0.52
1:A:907:LEU:HG	1:A:937:PRO:HA	1.91	0.52
1:A:185:PRO:HD2	1:A:188:ASP:OD2	2.09	0.52
1:A:96:GLN:NE2	1:A:98:TRP:C	2.67	0.52
1:A:114:LEU:N	1:A:117:GLU:OE2	2.40	0.52
1:A:319:LEU:HD23	1:A:442:ARG:HG2	1.91	0.52
1:A:470:LEU:H	1:A:470:LEU:HD23	1.75	0.52
1:A:388:PHE:O	1:A:388:PHE:CG	2.63	0.51
1:A:134:MET:HA	1:A:147:ASN:O	2.10	0.51
1:A:695:PRO:N	1:A:696:PRO:HD2	2.25	0.51
1:A:498:LEU:CD1	1:A:533:LEU:HD13	2.41	0.51
1:A:162:TYR:O	1:A:165:VAL:HG12	2.11	0.51
1:A:253:ALA:HB1	1:A:258:LEU:O	2.11	0.51
1:A:271:LEU:HD11	1:A:275:TYR:CE1	2.46	0.51
1:A:714:THR:N	1:A:715:PRO:HD2	2.25	0.51
1:A:400:ILE:HD12	1:A:406:LEU:HD23	1.92	0.51
1:A:692:MET:HE3	1:A:716:LEU:HD22	1.92	0.51
1:A:873:LEU:HD23	1:A:875:ILE:CG2	2.42	0.50
1:A:94:ASP:HB3	1:A:136:GLN:OE1	2.11	0.50
1:A:611:LEU:HD12	1:A:612:THR:HG23	1.93	0.50
1:A:527:ILE:HD11	1:A:529:MET:CE	2.40	0.50
1:A:903:ASP:CG	1:A:904:ASN:H	2.20	0.50
1:A:793:ILE:HB	1:A:811:LEU:HD11	1.93	0.50
1:A:25:MET:HE3	1:A:38:TYR:CD1	2.47	0.49
1:A:509:GLN:HG2	1:A:603:TYR:O	2.13	0.49
1:A:933:ALA:C	1:A:935:MET:N	2.70	0.49
1:A:100:ASN:HA	1:A:140:GLN:HB2	1.94	0.49
1:A:793:ILE:CD1	1:A:858:ILE:HD11	2.41	0.49
1:A:287:VAL:CG2	1:A:335:GLN:HG2	2.42	0.49
1:A:69:LEU:HD22	1:A:134:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HB3	1:A:92:PRO:HD3	1.95	0.49
1:A:514:LEU:HD21	1:A:574:LEU:HD21	1.94	0.48
1:A:396:THR:HG22	4:A:1313:HOH:O	2.13	0.48
1:A:453:GLU:O	1:A:454:GLN:C	2.55	0.48
1:A:70:ARG:HH22	1:A:88:LYS:CE	2.26	0.48
1:A:756:ASN:O	3:A:1202:AMP:N6	2.40	0.48
1:A:136:GLN:OE1	1:A:136:GLN:N	2.47	0.48
1:A:123:GLU:CD	1:A:123:GLU:H	2.21	0.48
1:A:887:HIS:HB2	1:A:926:PHE:CZ	2.49	0.48
1:A:897:LEU:O	1:A:907:LEU:HA	2.13	0.47
1:A:123:GLU:CD	1:A:123:GLU:N	2.72	0.47
1:A:482:ALA:HA	1:A:500:TYR:HB3	1.97	0.47
1:A:925:ARG:HA	1:A:928:GLN:HG2	1.97	0.47
1:A:45:THR:HG22	1:A:143:LYS:CD	2.45	0.47
1:A:746:SER:OG	1:A:748:LEU:HB2	2.14	0.47
1:A:359:GLU:CD	1:A:415:ARG:HH22	2.24	0.46
1:A:802:PRO:HD2	4:A:1321:HOH:O	2.16	0.46
1:A:687:VAL:HG22	1:A:701:TRP:CH2	2.51	0.46
1:A:99:ARG:HG2	1:A:100:ASN:H	1.80	0.46
1:A:672:TRP:HB2	1:A:764:VAL:HG11	1.98	0.46
1:A:873:LEU:O	1:A:874:ARG:HB3	2.16	0.46
1:A:99:ARG:O	1:A:100:ASN:C	2.59	0.46
1:A:150:HIS:HE1	1:A:388:PHE:CE1	2.34	0.46
1:A:529:MET:HE3	1:A:535:MET:HA	1.98	0.46
1:A:619:TYR:HE2	1:A:640:LEU:HD21	1.80	0.46
1:A:493:PHE:O	1:A:494:GLU:C	2.57	0.45
1:A:366:ASN:O	1:A:367:TYR:C	2.59	0.45
1:A:474:LEU:HD21	1:A:675:TRP:CG	2.51	0.45
1:A:903:ASP:CG	1:A:904:ASN:N	2.72	0.45
1:A:211:GLY:O	1:A:213:MET:HG2	2.15	0.45
1:A:115:GLN:HG3	1:A:116:THR:N	2.31	0.45
1:A:150:HIS:CE1	1:A:388:PHE:CE1	3.04	0.45
1:A:882:ALA:O	1:A:886:THR:HG23	2.16	0.45
1:A:43:LEU:HB3	1:A:385:VAL:HG13	1.99	0.45
1:A:282:LEU:HD23	1:A:357:LEU:O	2.16	0.45
1:A:388:PHE:C	1:A:390:GLU:H	2.24	0.45
1:A:883:VAL:O	1:A:886:THR:OG1	2.17	0.45
1:A:44:ILE:HB	1:A:144:PHE:HB3	1.98	0.45
1:A:161:ILE:HD11	1:A:301:VAL:HG11	1.99	0.45
1:A:498:LEU:HD13	1:A:533:LEU:HD13	1.99	0.45
1:A:93:TRP:H	1:A:131:ARG:HH22	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ASN:HA	4:A:1409:HOH:O	2.16	0.44
1:A:50:ILE:O	1:A:52:LEU:HD22	2.18	0.44
1:A:910:TYR:C	1:A:911:ILE:HD12	2.42	0.44
1:A:16:TYR:HA	1:A:17:PRO:HD3	1.88	0.44
1:A:171:ALA:HA	1:A:176:LYS:HG3	1.99	0.44
1:A:474:LEU:HD21	1:A:675:TRP:CD2	2.53	0.44
1:A:130:MET:O	1:A:131:ARG:C	2.60	0.44
1:A:37:ILE:HA	1:A:390:GLU:HG2	1.98	0.44
1:A:184:ARG:HD2	1:A:294:LEU:HD11	1.99	0.44
1:A:529:MET:CE	1:A:535:MET:HA	2.48	0.44
1:A:599:LYS:O	1:A:602:THR:HG23	2.18	0.43
1:A:34:ASP:OD1	1:A:34:ASP:N	2.52	0.43
1:A:51:ASN:OD1	1:A:54:VAL:HG23	2.18	0.43
1:A:868:VAL:HG13	1:A:871:ARG:HB2	2.01	0.43
1:A:184:ARG:HD2	1:A:294:LEU:CD1	2.48	0.43
1:A:388:PHE:C	1:A:390:GLU:N	2.76	0.43
1:A:474:LEU:HD11	1:A:675:TRP:HB3	2.01	0.43
1:A:153:LEU:HD13	1:A:158:MET:CE	2.48	0.43
1:A:120:GLN:O	1:A:123:GLU:CD	2.54	0.43
1:A:289:GLY:HA3	1:A:305:ILE:O	2.18	0.43
1:A:291:PRO:HB2	1:A:292:HIS:H	1.57	0.43
1:A:551:PRO:HB3	1:A:665:ILE:HG23	2.00	0.43
1:A:527:ILE:CG1	1:A:529:MET:HE2	2.45	0.43
1:A:508:ASN:O	1:A:512:HIS:HD2	2.01	0.43
1:A:25:MET:HE1	1:A:150:HIS:HB2	2.01	0.43
1:A:33:PRO:O	1:A:34:ASP:C	2.62	0.43
1:A:913:ARG:HD3	1:A:916:PRO:HA	2.01	0.43
1:A:530:GLU:CG	1:A:576:GLN:HE22	2.32	0.42
1:A:853:LEU:HB3	1:A:854:PRO:CD	2.48	0.42
1:A:913:ARG:NH2	1:A:918:LEU:O	2.52	0.42
1:A:535:MET:HE3	1:A:539:LEU:HD23	2.02	0.42
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.85	0.42
1:A:96:GLN:HE22	1:A:98:TRP:C	2.28	0.42
1:A:132:CYS:O	1:A:132:CYS:SG	2.76	0.42
1:A:94:ASP:OD1	1:A:136:GLN:NE2	2.52	0.42
1:A:98:TRP:CE3	1:A:99:ARG:O	2.64	0.42
1:A:654:THR:HB	1:A:655:PRO:CD	2.50	0.42
1:A:948:LEU:HD22	1:A:952:GLY:O	2.20	0.42
1:A:192:TRP:O	1:A:196:GLN:HG2	2.20	0.42
1:A:52:LEU:HD22	1:A:52:LEU:H	1.85	0.42
1:A:906:ARG:HE	1:A:906:ARG:HB2	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:O	1:A:220:VAL:N	2.53	0.41
1:A:25:MET:HB3	1:A:25:MET:HE2	1.82	0.41
1:A:325:GLN:HA	1:A:325:GLN:OE1	2.21	0.41
1:A:949:ASN:OD1	1:A:949:ASN:C	2.63	0.41
1:A:949:ASN:ND2	1:A:953:LYS:HB2	2.35	0.41
1:A:188:ASP:OD1	1:A:188:ASP:N	2.46	0.41
1:A:527:ILE:HD13	1:A:539:LEU:HD13	2.03	0.41
1:A:717:VAL:HA	1:A:720:ILE:HG12	2.03	0.41
1:A:65:ARG:NH2	1:A:181:PRO:O	2.54	0.41
1:A:141:THR:C	1:A:142:TYR:CG	2.98	0.41
1:A:539:LEU:HD12	1:A:549:TYR:CG	2.56	0.41
1:A:904:ASN:OD1	1:A:904:ASN:C	2.63	0.41
1:A:19:SER:O	1:A:20:PRO:C	2.63	0.41
1:A:388:PHE:O	1:A:390:GLU:N	2.53	0.41
1:A:620:VAL:HG22	1:A:634:LEU:HD23	2.02	0.41
1:A:732:ARG:HH11	1:A:732:ARG:HD2	1.68	0.41
1:A:153:LEU:HD13	1:A:158:MET:HE3	2.03	0.41
1:A:855:GLU:HB2	4:A:1437:HOH:O	2.21	0.40
1:A:422:GLU:O	1:A:425:ALA:HB3	2.21	0.40
1:A:131:ARG:O	1:A:132:CYS:C	2.64	0.40
1:A:907:LEU:O	1:A:937:PRO:CB	2.69	0.40
1:A:57:GLN:O	1:A:61:LYS:HG2	2.21	0.40
1:A:164:GLU:O	1:A:168:PHE:HD2	2.04	0.40
1:A:560:ARG:NE	4:A:1302:HOH:O	2.21	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	898/967 (93%)	821 (91%)	70 (8%)	7 (1%)	16 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	142	TYR
1	A	291	PRO
1	A	776	GLU
1	A	91	LEU
1	A	219	ARG
1	A	172	GLY

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	816/869 (94%)	771 (94%)	45 (6%)	19 45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	37	ILE
1	A	84	ILE
1	A	85	VAL
1	A	88	LYS
1	A	91	LEU
1	A	93	TRP
1	A	94	ASP
1	A	112	LEU
1	A	123	GLU
1	A	130	MET
1	A	131	ARG
1	A	133	LEU
1	A	134	MET
1	A	137	LEU
1	A	138	SER
1	A	290	ARG
1	A	295	SER

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Mol	Chain	Res	Type
1	A	311	ARG
1	A	330	LYS
1	A	363	VAL
1	A	396	THR
1	A	397	VAL
1	A	451	THR
1	A	494	GLU
1	A	501	GLN
1	A	539	LEU
1	A	602	THR
1	A	611	LEU
1	A	624	SER
1	A	640	LEU
1	A	709	VAL
1	A	746	SER
1	A	757	TYR
1	A	773	ASP
1	A	775	GLU
1	A	834	ILE
1	A	840	SER
1	A	898	ARG
1	A	905	GLN
1	A	906	ARG
1	A	908	VAL
1	A	922	GLU
1	A	935	MET
1	A	950	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	120	GLN
1	A	150	HIS
1	A	163	GLN
1	A	196	GLN
1	A	475	HIS
1	A	481	GLN
1	A	501	GLN
1	A	509	GLN
1	A	576	GLN
1	A	610	ASN

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Mol	Chain	Res	Type
1	A	866	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](#)

2 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	1.34	1 (16%)	5,10,10	1.28	1 (20%)
3	AMP	A	1202	-	25,25,25	0.56	0	37,38,38	0.59	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	-	-	0/8/8/8	-
3	AMP	A	1202	-	-	5/10/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	LEU	O-C	3.13	1.31	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	LEU	OXT-C-O	2.85	130.54	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

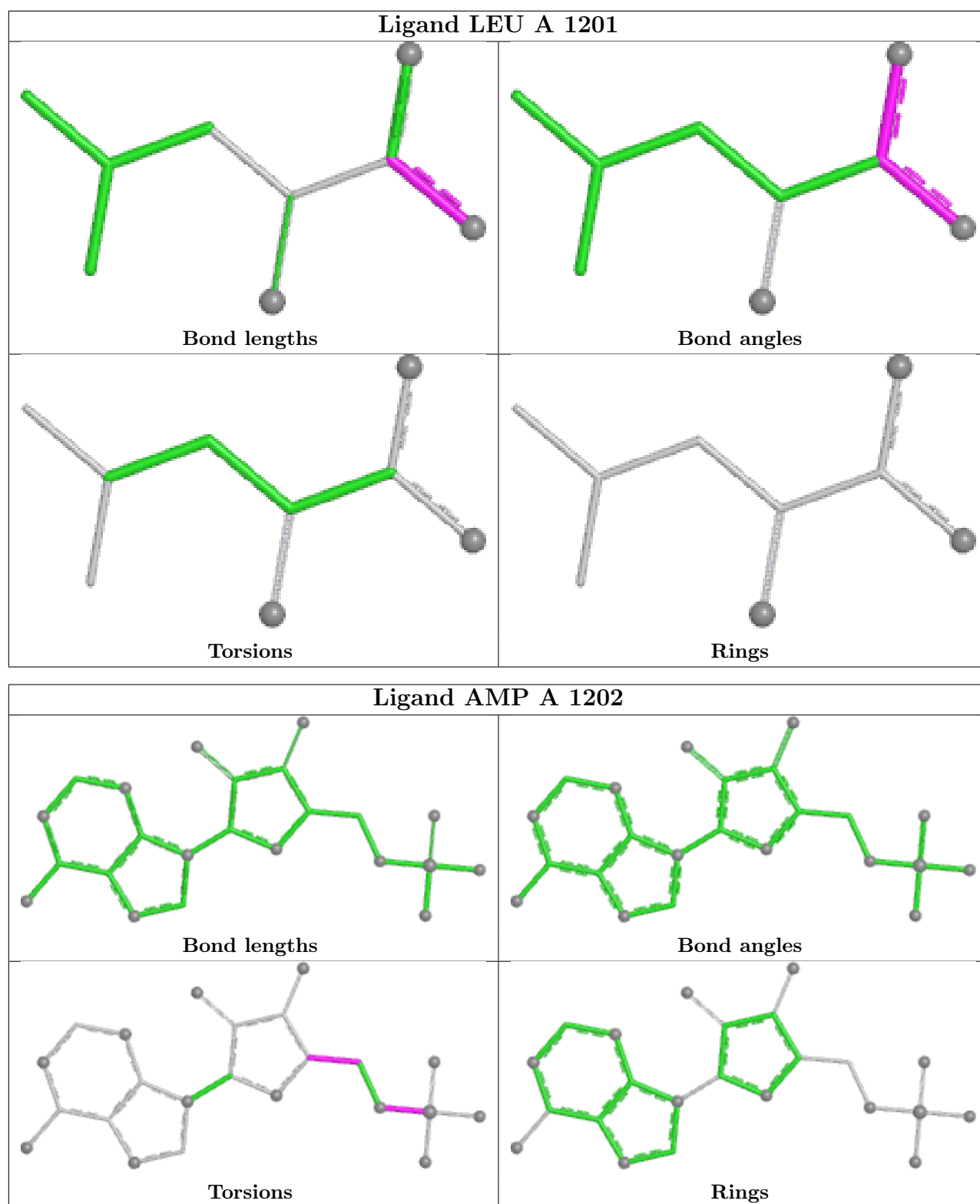
Mol	Chain	Res	Type	Atoms
3	A	1202	AMP	C5'-O5'-P-O2P
3	A	1202	AMP	C5'-O5'-P-O3P
3	A	1202	AMP	C3'-C4'-C5'-O5'
3	A	1202	AMP	O4'-C4'-C5'-O5'
3	A	1202	AMP	C5'-O5'-P-O1P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	LEU	1	0
3	A	1202	AMP	1	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 ⓘ

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 ⓘ

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	910/967 (94%)	-0.00	65 (7%) 22 19	26, 61, 132, 226	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	MET	7.2
1	A	92	PRO	7.0
1	A	93	TRP	6.6
1	A	900	ASP	6.3
1	A	594	ASP	6.1
1	A	129	LEU	6.0
1	A	775	GLU	4.8
1	A	904	ASN	4.6
1	A	367	TYR	4.6
1	A	154	ASP	4.6
1	A	296	GLY	4.5
1	A	95	TYR	4.2
1	A	112	LEU	4.1
1	A	132	CYS	4.0
1	A	128	PRO	3.8
1	A	94	ASP	3.8
1	A	91	LEU	3.8
1	A	901	THR	3.7
1	A	142	TYR	3.6
1	A	903	ASP	3.5
1	A	124	PHE	3.5
1	A	141	THR	3.4
1	A	131	ARG	3.3
1	A	294	LEU	3.3
1	A	841	GLY	3.3
1	A	90	ASP	3.3
1	A	135	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	385	VAL	3.2
1	A	171	ALA	3.1
1	A	384	ASP	3.0
1	A	89	VAL	3.0
1	A	933	ALA	2.9
1	A	297	VAL	2.9
1	A	906	ARG	2.9
1	A	388	PHE	2.9
1	A	907	LEU	2.9
1	A	118	ARG	2.9
1	A	934	TYR	2.8
1	A	133	LEU	2.8
1	A	156	TRP	2.8
1	A	88	LYS	2.7
1	A	186	TYR	2.7
1	A	295	SER	2.7
1	A	127	ALA	2.6
1	A	134	MET	2.5
1	A	223	LEU	2.5
1	A	16	TYR	2.5
1	A	126	VAL	2.4
1	A	155	GLY	2.4
1	A	232	PRO	2.4
1	A	599	LYS	2.4
1	A	366	ASN	2.4
1	A	187	GLN	2.4
1	A	870	LEU	2.3
1	A	905	GLN	2.3
1	A	98	TRP	2.3
1	A	292	HIS	2.3
1	A	15	ILE	2.2
1	A	899	GLU	2.2
1	A	290	ARG	2.2
1	A	914	LYS	2.1
1	A	138	SER	2.1
1	A	173	ILE	2.1
1	A	119	GLN	2.0
1	A	47	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

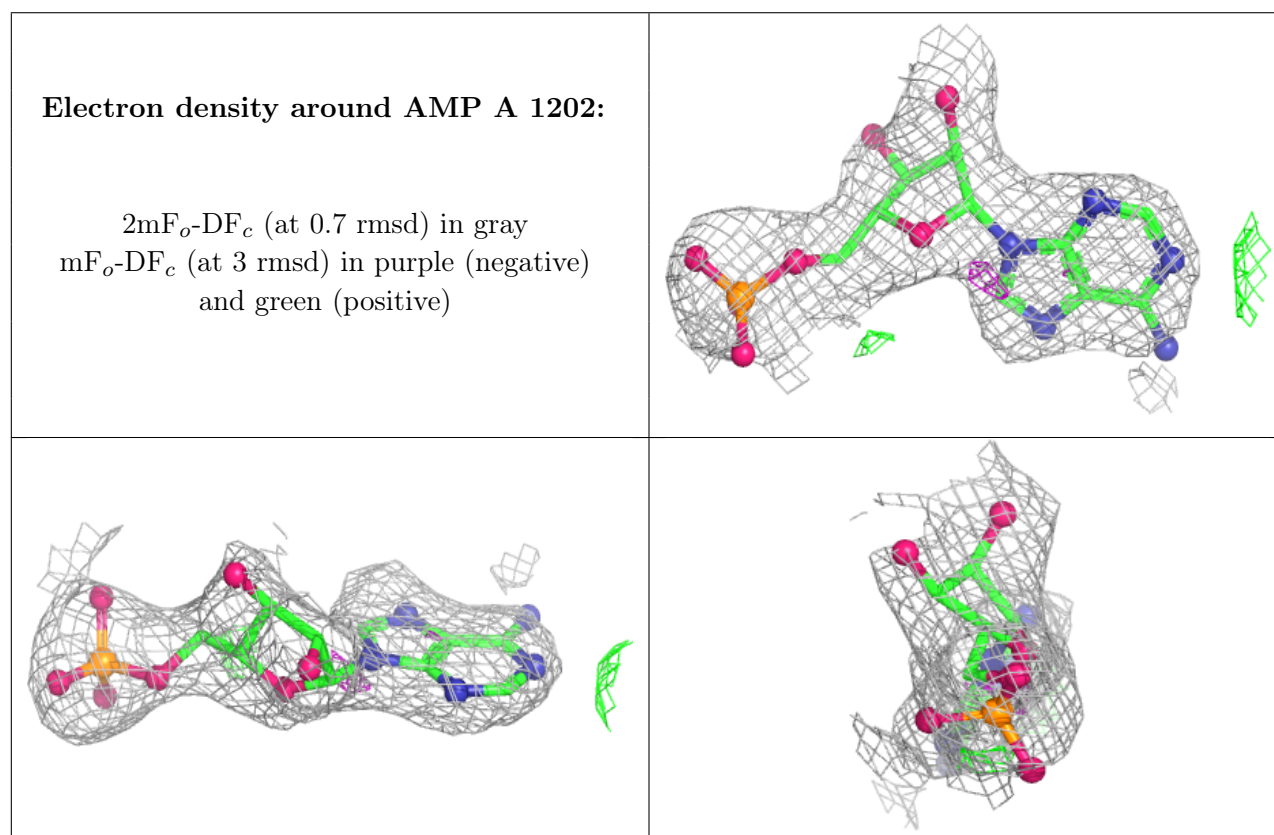
There are no oligosaccharides in this entry.

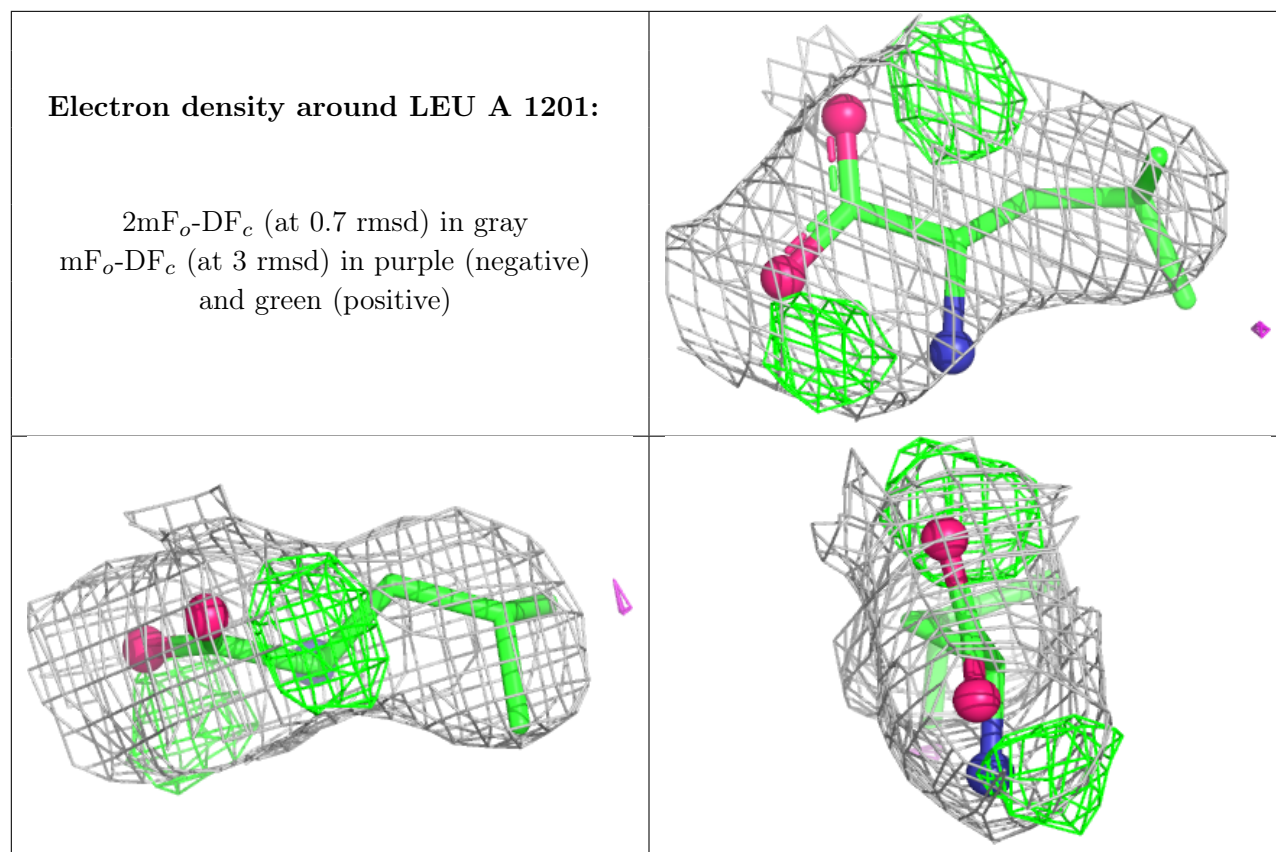
6.4 Ligands [i](#)

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
3	AMP	A	1202	23/23	0.90	0.11	42,70,82,84	3
2	LEU	A	1201	9/9	0.94	0.13	39,61,67,68	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.