



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:11 PM UTC

PDB ID : 8YLW / pdb_00008ylw
Title : Crystal Structure of Lysyl-tRNA Synthetase from Plasmodium falciparum complexed with Lys-AMS
Authors : Sharma, V.K.; Manickam, Y.; Bagale, S.; Pradeepkumar, P.I.; Sharma, A.
Deposited on : 2024-03-07
Resolution : 2.50 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

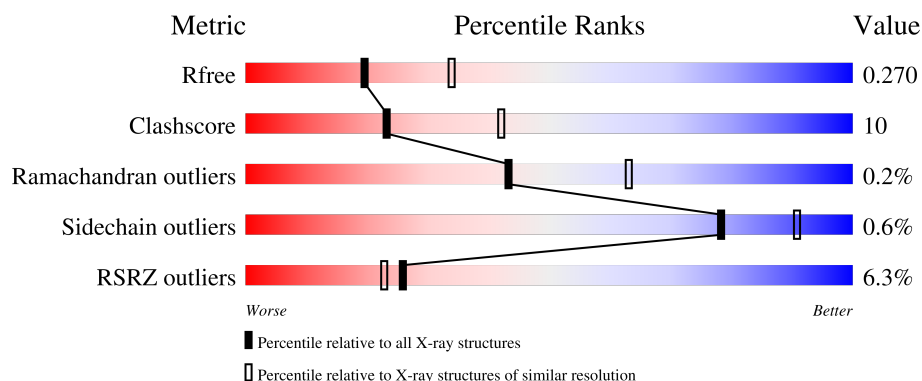
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	507	4% 75% 20% • •
1	B	507	3% 76% 19% • •
1	C	507	4% 72% 21% • 6%
1	D	507	13% 67% 25% • 5%

2 Entry composition [i](#)

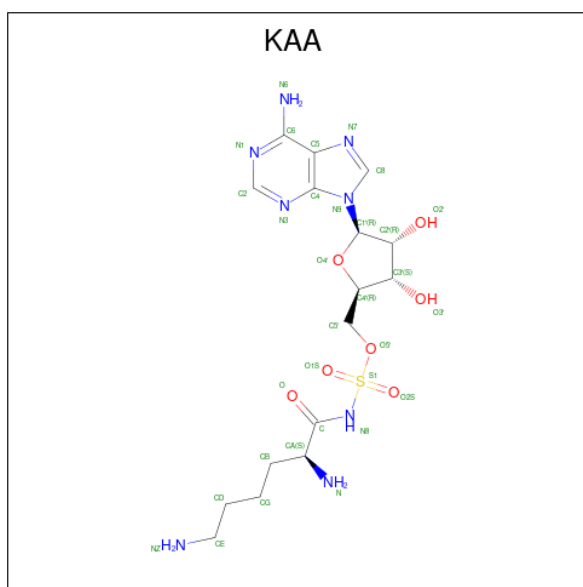
There are 3 unique types of molecules in this entry. The entry contains 15701 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	487	Total	C	N	O	S	0	0	0
			3939	2538	656	728	17			
1	A	486	Total	C	N	O	S	0	0	0
			3914	2527	650	720	17			
1	D	483	Total	C	N	O	S	0	0	0
			3756	2420	632	688	16			
1	C	479	Total	C	N	O	S	0	0	0
			3804	2459	631	697	17			

- Molecule 2 is 5'-O-[(L-LYSYLAMINO)SULFONYL]ADENOSINE (CCD ID: KAA) (formula: C₁₆H₂₆N₈O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
2	A	1	Total	C	N	O	S	0	0
			32	16	8	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
2	C	1	Total	C	N	O	S	0	0
			32	16	8	7	1		

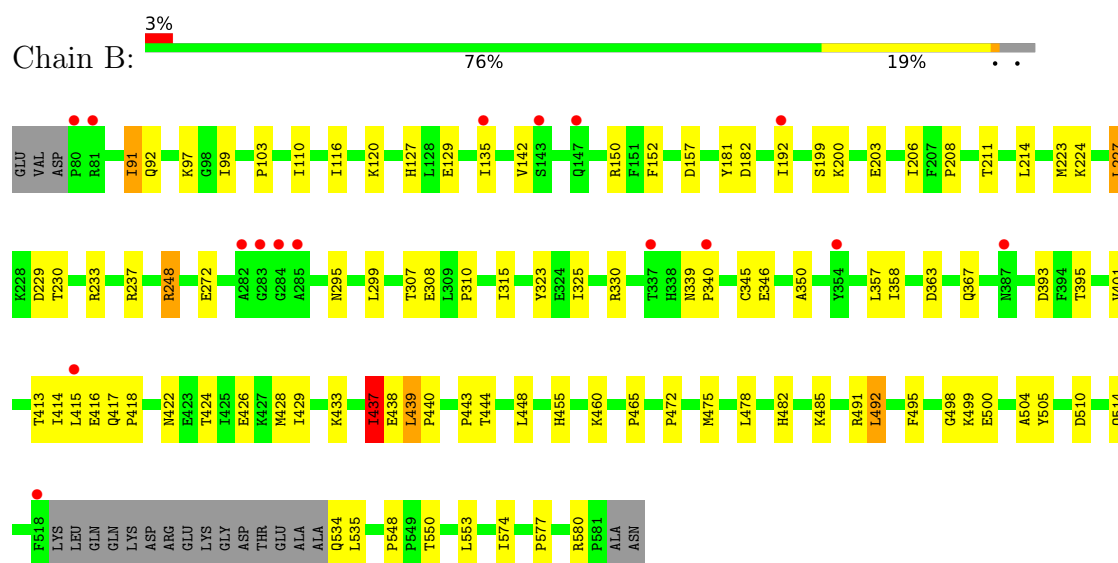
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	57	Total	O	0	0
			57	57		
3	A	50	Total	O	0	1
			50	50		
3	D	19	Total	O	0	0
			19	19		
3	C	34	Total	O	0	0
			34	34		

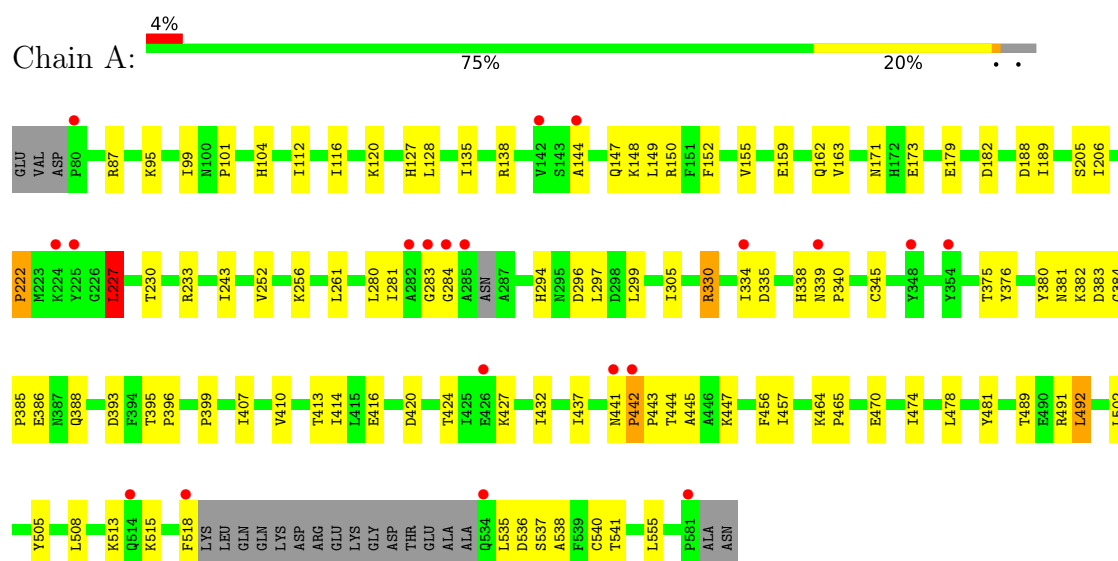
3 Residue-property plots

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 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.

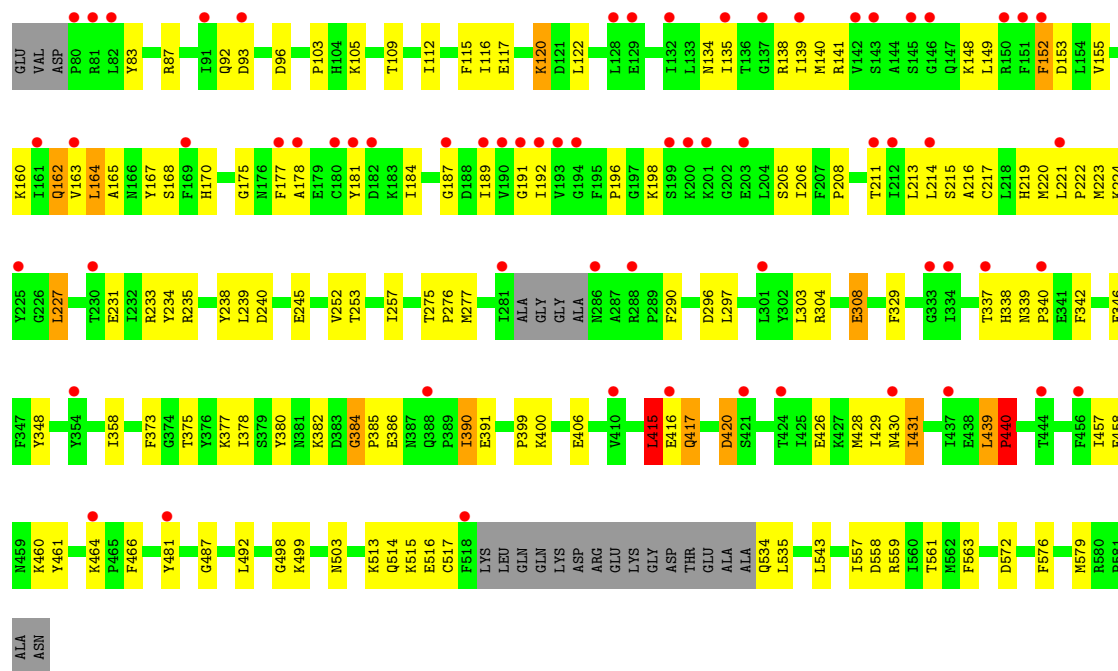
• Molecule 1: Lysine–tRNA ligase



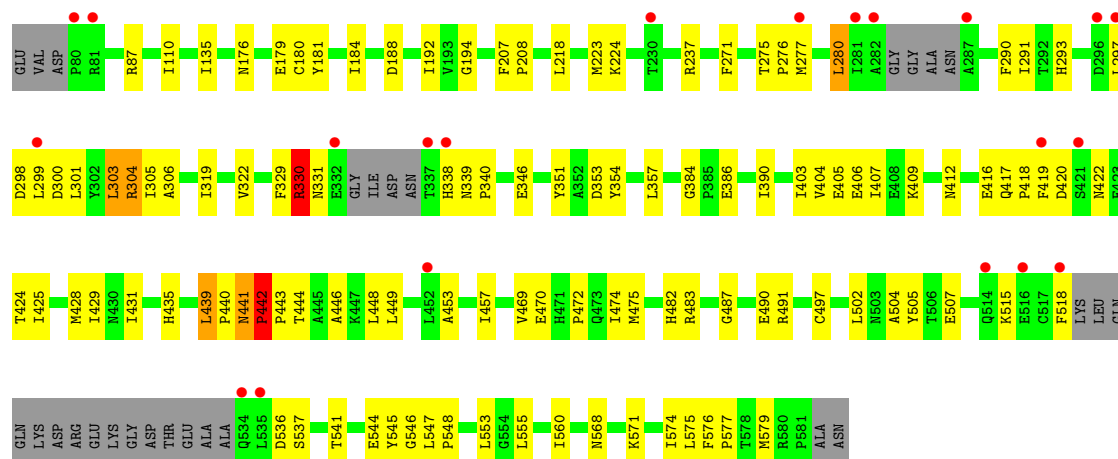
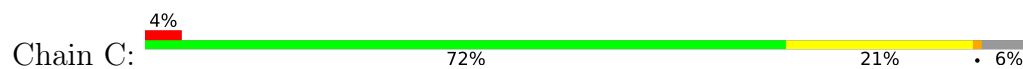
• Molecule 1: Lysine–tRNA ligase



• Molecule 1: Lysine–tRNA ligase



• Molecule 1: Lysine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	59.36Å 302.19Å 141.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.53 – 2.50 45.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.53-2.50) 99.9 (45.53-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.15rc1_3423-0000)	Depositor
R, R_{free}	0.209 , 0.267 0.220 , 0.270	Depositor DCC
R_{free} test set	4479 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15701	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.61% 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: KAA

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	1.06	43/4011 (1.1%)	0.81	9/5426 (0.2%)
1	B	0.80	16/4037 (0.4%)	0.77	3/5459 (0.1%)
1	C	0.89	24/3901 (0.6%)	0.91	9/5284 (0.2%)
1	D	0.98	13/3849 (0.3%)	1.04	22/5221 (0.4%)
All	All	0.94	96/15798 (0.6%)	0.89	43/21390 (0.2%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	PRO	C-O	-10.28	1.16	1.24
1	A	396	PRO	CA-C	-9.89	1.45	1.52
1	A	399	PRO	C-O	-8.25	1.14	1.23
1	B	500	GLU	C-O	-8.15	1.14	1.23
1	B	492	LEU	C-O	-7.98	1.14	1.23
1	A	284	GLY	C-O	-7.85	1.18	1.24
1	A	381	ASN	CA-C	-7.75	1.43	1.52
1	A	492	LEU	C-O	-7.66	1.14	1.23
1	A	538	ALA	C-O	-7.46	1.15	1.24
1	D	227	LEU	N-CA	-7.21	1.36	1.46
1	A	388	GLN	CA-C	-7.11	1.44	1.53
1	B	295	ASN	CA-C	-7.10	1.44	1.52
1	B	248	ARG	C-O	-7.09	1.15	1.24
1	B	499	LYS	C-O	-7.00	1.15	1.24
1	A	104	HIS	C-O	-6.98	1.15	1.24
1	C	330	ARG	C-O	-6.97	1.16	1.23
1	C	305	ILE	C-O	-6.89	1.17	1.24
1	C	338	HIS	CA-C	-6.86	1.44	1.52
1	A	540	CYS	C-O	-6.80	1.16	1.24
1	A	393	ASP	C-O	-6.72	1.16	1.24
1	D	377	LYS	C-O	-6.71	1.16	1.24
1	C	180	CYS	C-O	-6.65	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	ARG	C-O	-6.53	1.15	1.24
1	D	514	GLN	N-CA	-6.47	1.38	1.46
1	C	291	ILE	C-O	-6.41	1.16	1.24
1	D	162	GLN	C-O	-6.39	1.16	1.23
1	D	514	GLN	CA-C	-6.35	1.44	1.52
1	A	383	ASP	CA-C	-6.35	1.45	1.53
1	D	377	LYS	CA-C	-6.30	1.45	1.52
1	B	229	ASP	CA-C	-6.30	1.44	1.52
1	A	280	LEU	C-O	-6.27	1.15	1.24
1	A	442	PRO	C-O	-6.24	1.17	1.24
1	C	293	HIS	C-O	-6.24	1.16	1.24
1	C	306	ALA	C-O	-6.20	1.17	1.23
1	C	439	LEU	CA-C	-6.18	1.44	1.52
1	D	224	LYS	C-O	-6.15	1.17	1.24
1	A	179	GLU	CA-C	-6.14	1.44	1.52
1	C	304	ARG	C-O	-6.12	1.16	1.23
1	D	417	GLN	CA-C	-6.08	1.46	1.53
1	A	281	ILE	CA-C	-6.05	1.44	1.52
1	A	104	HIS	CA-C	-6.04	1.44	1.52
1	B	437	ILE	C-O	-5.98	1.17	1.24
1	A	330	ARG	C-O	-5.92	1.17	1.23
1	A	384	GLY	C-O	-5.91	1.16	1.24
1	A	537	SER	C-O	-5.89	1.16	1.24
1	A	396	PRO	CA-CB	-5.88	1.49	1.54
1	C	303	LEU	C-O	-5.88	1.16	1.23
1	D	415	LEU	CA-C	-5.87	1.45	1.52
1	C	409	LYS	CA-C	-5.84	1.45	1.52
1	A	395	THR	C-O	-5.84	1.16	1.24
1	A	441	ASN	CA-C	-5.79	1.45	1.52
1	D	178	ALA	C-O	-5.77	1.17	1.24
1	A	541	THR	C-O	-5.74	1.17	1.24
1	D	170	HIS	C-O	-5.74	1.17	1.24
1	C	303	LEU	CA-C	-5.64	1.45	1.52
1	B	157	ASP	C-O	-5.63	1.16	1.23
1	A	381	ASN	C-O	-5.61	1.16	1.23
1	A	443	PRO	CA-C	-5.61	1.48	1.53
1	A	222	PRO	C-O	-5.59	1.17	1.23
1	A	393	ASP	CA-C	-5.57	1.46	1.52
1	A	388	GLN	C-O	-5.55	1.16	1.23
1	D	464	LYS	C-O	-5.49	1.18	1.24
1	B	438	GLU	CA-C	-5.48	1.45	1.52
1	A	384	GLY	C-N	-5.48	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	THR	C-O	-5.45	1.16	1.23
1	A	447	LYS	C-O	-5.39	1.17	1.24
1	C	297	LEU	C-O	-5.39	1.16	1.24
1	A	442	PRO	CA-C	-5.39	1.47	1.52
1	A	383	ASP	N-CA	-5.36	1.40	1.46
1	A	385	PRO	C-O	-5.33	1.18	1.23
1	C	223	MET	CA-C	-5.32	1.46	1.53
1	B	92	GLN	C-O	-5.28	1.17	1.24
1	A	540	CYS	CA-C	-5.28	1.46	1.52
1	A	536	ASP	C-O	-5.26	1.17	1.23
1	C	330	ARG	CA-C	-5.25	1.46	1.52
1	B	227	LEU	CA-C	-5.21	1.46	1.53
1	C	442	PRO	CA-C	-5.19	1.47	1.52
1	C	304	ARG	CA-C	-5.15	1.46	1.52
1	C	409	LYS	C-O	-5.15	1.18	1.24
1	A	540	CYS	N-CA	-5.13	1.40	1.46
1	C	299	LEU	C-O	-5.13	1.17	1.23
1	C	180	CYS	N-CA	-5.11	1.40	1.46
1	A	179	GLU	C-O	-5.11	1.18	1.24
1	B	157	ASP	CG-OD1	-5.10	1.15	1.25
1	B	498	GLY	C-O	-5.08	1.16	1.23
1	C	280	LEU	C-O	-5.07	1.17	1.24
1	C	441	ASN	CA-C	-5.07	1.46	1.52
1	C	223	MET	N-CA	-5.07	1.39	1.45
1	A	330	ARG	CA-C	-5.05	1.46	1.52
1	A	445	ALA	C-O	-5.05	1.18	1.24
1	C	300	ASP	N-CA	-5.04	1.40	1.46
1	D	515	LYS	C-O	-5.03	1.18	1.24
1	B	91	ILE	C-O	-5.03	1.18	1.24
1	A	386	GLU	CA-CB	-5.03	1.46	1.53
1	A	179	GLU	C-N	-5.01	1.27	1.33
1	B	438	GLU	C-O	-5.00	1.17	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	439	LEU	CA-C-N	24.14	144.62	119.76
1	C	439	LEU	C-N-CA	24.14	144.62	119.76
1	D	439	LEU	CA-C-N	21.51	146.72	119.84
1	D	439	LEU	C-N-CA	21.51	146.72	119.84
1	A	442	PRO	N-CA-C	-15.33	92.00	110.70
1	B	439	LEU	CA-C-N	14.32	137.74	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	LEU	C-N-CA	14.32	137.74	119.84
1	D	384	GLY	CA-C-N	13.84	134.42	119.05
1	D	384	GLY	C-N-CA	13.84	134.42	119.05
1	C	442	PRO	N-CA-C	-12.21	95.80	110.70
1	D	175	GLY	N-CA-C	11.34	122.72	111.95
1	A	395	THR	CA-C-N	9.54	126.53	119.66
1	A	395	THR	C-N-CA	9.54	126.53	119.66
1	D	517	CYS	N-CA-C	7.86	119.93	111.36
1	D	431	ILE	CB-CA-C	-7.29	100.85	112.16
1	A	227	LEU	N-CA-C	7.10	120.81	112.72
1	D	308	GLU	N-CA-C	6.72	119.46	111.33
1	C	298	ASP	N-CA-C	6.68	120.45	111.24
1	A	441	ASN	CA-C-N	-6.45	113.73	120.38
1	A	441	ASN	C-N-CA	-6.45	113.73	120.38
1	B	295	ASN	N-CA-C	6.42	118.16	111.03
1	D	416	GLU	N-CA-C	6.20	118.20	108.96
1	D	464	LYS	CB-CA-C	-6.12	100.48	109.97
1	D	170	HIS	N-CA-C	5.85	118.19	109.59
1	D	516	GLU	N-CA-C	5.85	118.44	111.71
1	D	181	TYR	N-CA-C	5.63	119.99	113.18
1	A	281	ILE	CB-CA-C	-5.61	102.84	111.31
1	D	439	LEU	C-N-CD	-5.60	102.03	125.00
1	D	440	PRO	CA-C-N	-5.53	113.69	119.83
1	D	440	PRO	C-N-CA	-5.53	113.69	119.83
1	C	536	ASP	N-CA-C	5.53	117.81	109.41
1	D	152	PHE	CB-CA-C	-5.49	98.62	111.09
1	C	331	ASN	N-CA-C	5.49	117.85	109.62
1	C	439	LEU	C-N-CD	-5.46	102.64	125.00
1	A	441	ASN	N-CA-C	5.44	121.83	109.81
1	C	224	LYS	N-CA-C	5.38	117.15	111.28
1	C	338	HIS	CB-CA-C	-5.36	98.50	109.38
1	D	378	ILE	CB-CA-C	-5.32	102.94	110.82
1	A	399	PRO	CB-CA-C	-5.27	104.20	111.21
1	D	227	LEU	N-CA-C	-5.18	107.51	113.88
1	D	120	LYS	N-CA-C	5.02	118.66	112.54
1	D	92	GLN	CA-C-N	-5.01	112.37	121.14
1	D	92	GLN	C-N-CA	-5.01	112.37	121.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3914	0	3828	59	0
1	B	3939	0	3865	68	0
1	C	3804	0	3641	89	0
1	D	3756	0	3549	107	0
2	A	32	0	26	0	0
2	B	32	0	26	5	0
2	C	32	0	26	3	0
2	D	32	0	26	3	0
3	A	50	0	0	0	0
3	B	57	0	0	1	0
3	C	34	0	0	0	0
3	D	19	0	0	0	0
All	All	15701	0	14987	314	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 10.

All (314) 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:C:441:ASN:CB	1:C:442:PRO:HD3	1.69	1.20
1:C:441:ASN:CB	1:C:442:PRO:CD	2.47	0.92
1:D:428:MET:HA	1:D:431:ILE:HD12	1.53	0.90
1:B:437:ILE:CD1	1:B:455:HIS:CD2	2.54	0.90
1:B:437:ILE:CD1	1:B:455:HIS:CG	2.56	0.89
1:C:412:ASN:ND2	1:C:412:ASN:O	2.07	0.87
1:B:437:ILE:HD11	1:B:455:HIS:CD2	2.13	0.83
1:D:164:LEU:O	1:D:208:PRO:HD2	1.82	0.80
1:A:492:LEU:HD23	1:A:492:LEU:N	1.97	0.79
1:C:330:ARG:HG2	1:C:330:ARG:HH11	1.47	0.78
1:C:439:LEU:CB	1:C:440:PRO:HD2	2.13	0.77
1:B:437:ILE:HD13	1:B:455:HIS:CD2	2.18	0.77
1:B:315:ILE:HG21	1:B:550:THR:HG21	1.67	0.76
1:A:171:ASN:OD1	1:A:173:GLU:HB3	1.86	0.76
1:A:407:ILE:HG13	1:A:457:ILE:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:SER:HB2	1:B:203:GLU:H	1.53	0.74
1:D:189:ILE:HD11	1:D:215:SER:HB3	1.67	0.73
1:D:122:LEU:HB2	1:D:198:LYS:HD2	1.69	0.73
1:B:437:ILE:HD11	1:B:455:HIS:CE1	2.24	0.73
1:C:357:LEU:HD13	1:C:504:ALA:HB1	1.70	0.73
1:C:469:VAL:HG12	1:C:470:GLU:HG3	1.71	0.72
1:C:515:LYS:HA	1:C:518:PHE:HE2	1.54	0.72
1:B:437:ILE:HD11	1:B:455:HIS:CG	2.22	0.72
1:D:116:ILE:O	1:D:120:LYS:HB3	1.90	0.72
1:D:386:GLU:CD	1:D:386:GLU:H	1.98	0.71
1:D:420:ASP:OD1	1:D:420:ASP:N	2.22	0.71
1:B:580:ARG:HG3	1:A:297:LEU:HD22	1.72	0.70
1:C:547:LEU:HD12	1:C:548:PRO:HD2	1.74	0.70
1:D:148:LYS:HB3	1:D:167:TYR:HB2	1.74	0.69
1:C:507:GLU:OE1	2:C:601:KAA:NZ	2.25	0.69
1:C:181:TYR:HA	1:C:184:ILE:HD12	1.74	0.69
1:B:346:GLU:CD	2:B:601:KAA:HB1	2.18	0.68
1:D:390:ILE:HD12	1:D:390:ILE:O	1.94	0.67
1:D:406:GLU:HG2	1:D:457:ILE:CG2	2.25	0.67
1:D:164:LEU:C	1:D:164:LEU:HD23	2.20	0.67
1:D:426:GLU:O	1:D:430:ASN:N	2.24	0.67
1:D:337:THR:HG21	1:D:499:LYS:HD2	1.74	0.66
1:D:277:MET:HA	1:D:304:ARG:HD3	1.76	0.66
1:D:386:GLU:OE1	1:D:386:GLU:N	2.27	0.66
1:D:192:ILE:HG12	1:D:211:THR:HG22	1.78	0.65
1:B:135:ILE:HG12	1:B:206:ILE:HD13	1.78	0.65
1:C:277:MET:HE2	1:C:304:ARG:NH2	2.12	0.65
1:C:330:ARG:HH11	1:C:330:ARG:CG	2.09	0.65
1:A:334:ILE:O	1:A:334:ILE:HG13	1.97	0.64
1:C:504:ALA:HB2	1:C:553:LEU:HG	1.79	0.64
1:C:422:ASN:HA	1:C:425:ILE:HB	1.80	0.63
1:C:444:THR:O	1:C:448:LEU:HD12	1.98	0.63
1:B:437:ILE:HD11	1:B:455:HIS:NE2	2.14	0.63
1:A:515:LYS:HA	1:A:518:PHE:HE2	1.63	0.63
1:D:390:ILE:HD12	1:D:390:ILE:C	2.22	0.63
1:D:576:PHE:HB2	1:C:276:PRO:HD3	1.81	0.63
1:A:432:ILE:HG23	1:A:437:ILE:HB	1.82	0.62
1:D:557:ILE:O	1:D:561:THR:HG23	1.99	0.62
1:D:406:GLU:HG2	1:D:457:ILE:HG21	1.82	0.62
1:B:422:ASN:O	1:B:426:GLU:HG2	2.01	0.61
1:B:416:GLU:H	1:B:424:THR:HG21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:CG2	1:A:206:ILE:HD13	2.31	0.61
1:D:234:TYR:HB3	1:D:579:MET:HE3	1.82	0.61
1:D:192:ILE:HG23	1:D:208:PRO:HB3	1.82	0.60
1:B:429:ILE:HG22	1:B:433:LYS:HE2	1.83	0.60
1:D:217:CYS:SG	1:D:221:LEU:HD11	2.41	0.60
1:C:417:GLN:HE22	1:C:487:GLY:HA3	1.67	0.60
1:C:87:ARG:NH2	1:C:188:ASP:OD1	2.35	0.60
1:C:419:PHE:HB2	1:C:474:ILE:HD13	1.84	0.60
1:D:162:GLN:HB3	1:D:205:SER:HB2	1.84	0.59
1:D:308:GLU:HG3	1:D:348:TYR:OH	2.02	0.59
1:A:87:ARG:NH2	1:A:188:ASP:OD1	2.36	0.59
1:A:491:ARG:HA	1:A:505:TYR:HB3	1.85	0.59
1:D:152:PHE:HB2	1:D:163:VAL:HB	1.83	0.59
1:A:492:LEU:HD23	1:A:492:LEU:H	1.65	0.58
1:D:252:VAL:HA	1:C:271:PHE:CZ	2.38	0.58
1:C:277:MET:HA	1:C:304:ARG:HD3	1.85	0.58
1:A:416:GLU:O	1:A:424:THR:HG21	2.04	0.58
1:D:93:ASP:HA	1:D:96:ASP:HB2	1.83	0.58
1:D:296:ASP:O	1:D:297:LEU:HD23	2.03	0.58
1:C:420:ASP:OD1	1:C:420:ASP:N	2.33	0.58
1:D:148:LYS:O	1:D:177:PHE:CZ	2.57	0.57
1:D:460:LYS:HG2	1:D:461:TYR:CD2	2.40	0.57
2:D:601:KAA:O2S	2:D:601:KAA:H3'	2.03	0.57
1:D:148:LYS:HD3	1:D:167:TYR:HB3	1.87	0.57
1:B:150:ARG:NH2	1:B:182:ASP:OD2	2.33	0.57
1:D:83:TYR:O	1:D:87:ARG:HG2	2.04	0.57
1:C:453:ALA:HA	1:C:457:ILE:HD12	1.87	0.57
1:B:230:THR:HA	1:B:233:ARG:HE	1.70	0.57
1:C:237:ARG:NE	1:C:575:LEU:O	2.31	0.57
1:D:358:ILE:HD13	1:D:492:LEU:HD13	1.85	0.57
1:D:503:ASN:HD22	2:D:601:KAA:HN8	1.52	0.57
1:B:97:LYS:HB2	1:B:99:ILE:HD12	1.87	0.56
1:B:548:PRO:O	1:B:550:THR:HG23	2.05	0.56
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.86	0.56
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.86	0.56
1:D:103:PRO:HD2	1:D:214:LEU:HA	1.87	0.56
1:C:277:MET:HG2	1:C:329:PHE:HE1	1.70	0.56
1:D:112:ILE:O	1:D:116:ILE:HG13	2.05	0.56
1:C:425:ILE:O	1:C:429:ILE:HG13	2.06	0.56
1:B:350:ALA:HA	1:B:550:THR:HG22	1.88	0.56
1:D:155:VAL:HG12	1:D:160:LYS:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HG2	1:A:243:ILE:HD13	1.87	0.56
1:A:410:VAL:HG21	1:A:456:PHE:HB3	1.88	0.55
1:A:413:THR:O	1:A:414:ILE:HD13	2.05	0.55
1:D:559:ARG:O	1:D:563:PHE:HD2	1.89	0.55
1:D:234:TYR:CB	1:D:579:MET:HE3	2.36	0.55
1:D:415:LEU:HD11	1:D:428:MET:HG2	1.89	0.55
1:A:502:LEU:HB3	1:A:555:LEU:HD23	1.89	0.54
1:D:303:LEU:HB3	1:D:329:PHE:CD1	2.43	0.54
1:C:449:LEU:HB3	1:C:475:MET:HE3	1.90	0.54
1:D:148:LYS:HD3	1:D:167:TYR:CB	2.37	0.54
1:C:330:ARG:CG	1:C:330:ARG:NH1	2.69	0.54
1:D:457:ILE:O	1:D:460:LYS:N	2.38	0.54
1:D:109:THR:HG23	1:D:134:ASN:HB2	1.91	0.53
1:D:417:GLN:HE22	1:D:487:GLY:HA3	1.73	0.53
1:C:482:HIS:HA	1:C:490:GLU:HG3	1.90	0.53
1:D:252:VAL:HA	1:C:271:PHE:HZ	1.74	0.53
1:B:339:ASN:OD1	1:B:340:PRO:HD2	2.09	0.53
1:D:83:TYR:CD2	1:D:220:MET:HE2	2.45	0.52
1:C:417:GLN:NE2	1:C:487:GLY:HA3	2.25	0.52
1:A:283:GLY:HA3	1:A:305:ILE:HG12	1.92	0.52
1:D:481:TYR:CE1	1:D:513:LYS:HE3	2.44	0.52
1:C:277:MET:HE2	1:C:304:ARG:CZ	2.39	0.52
1:B:393:ASP:OD1	1:B:395:THR:OG1	2.21	0.52
1:D:139:ILE:O	1:D:187:GLY:N	2.36	0.52
1:B:510:ASP:OD2	1:A:95:LYS:NZ	2.42	0.52
1:B:272:GLU:HB2	1:B:323:TYR:CZ	2.45	0.52
1:C:416:GLU:H	1:C:424:THR:HG21	1.75	0.52
1:D:431:ILE:O	1:D:431:ILE:HG22	2.10	0.52
1:D:189:ILE:CD1	1:D:215:SER:HB3	2.38	0.52
1:A:481:TYR:CE2	1:A:513:LYS:HE3	2.45	0.51
1:D:213:LEU:HD21	1:D:216:ALA:HB2	1.92	0.51
1:B:574:ILE:O	1:B:577:PRO:HD3	2.09	0.51
1:C:428:MET:SD	1:C:449:LEU:HD12	2.50	0.51
1:A:173:GLU:O	1:A:173:GLU:HG3	2.11	0.51
1:D:426:GLU:O	1:D:429:ILE:N	2.43	0.51
1:D:148:LYS:HB3	1:D:167:TYR:CB	2.41	0.51
1:C:403:ILE:O	1:C:407:ILE:HG13	2.11	0.51
1:C:439:LEU:CB	1:C:440:PRO:CD	2.69	0.51
1:B:248:ARG:NH1	3:B:704:HOH:O	2.44	0.51
1:D:253:THR:O	1:D:257:ILE:HG13	2.11	0.50
1:D:346:GLU:CD	2:D:601:KAA:HB1	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:THR:O	1:B:448:LEU:HG	2.11	0.50
1:A:150:ARG:NH1	1:A:182:ASP:OD1	2.44	0.50
1:A:294:HIS:HE1	1:A:296:ASP:HB3	1.75	0.50
1:B:482:HIS:CE1	1:B:485:LYS:HG3	2.47	0.50
1:D:222:PRO:HD2	1:D:239:LEU:HD22	1.95	0.49
1:D:380:TYR:CE1	1:D:563:PHE:HA	2.47	0.49
1:B:478:LEU:HD21	1:B:535:LEU:HD11	1.94	0.49
1:A:147:GLN:O	1:A:147:GLN:HG3	2.13	0.49
1:D:275:THR:HB	1:D:276:PRO:HD2	1.93	0.49
1:C:515:LYS:HA	1:C:518:PHE:CE2	2.43	0.49
1:D:148:LYS:O	1:D:177:PHE:HZ	1.94	0.49
1:B:142:VAL:HG22	1:B:152:PHE:CD2	2.48	0.49
1:D:390:ILE:C	1:D:390:ILE:CD1	2.85	0.49
1:C:449:LEU:HD21	1:C:472:PRO:HG2	1.95	0.49
1:C:431:ILE:HD11	1:C:435:HIS:CE1	2.48	0.49
1:B:437:ILE:HD11	1:B:455:HIS:ND1	2.27	0.49
1:D:342:PHE:HB2	1:D:558:ASP:OD1	2.12	0.49
1:D:458:GLU:O	1:D:498:GLY:HA2	2.13	0.49
1:C:384:GLY:HA2	1:C:568:ASN:OD1	2.13	0.49
1:B:417:GLN:HA	1:B:418:PRO:C	2.38	0.49
1:D:152:PHE:CZ	1:D:184:ILE:HD11	2.48	0.48
1:D:115:PHE:CE2	1:D:196:PRO:HB3	2.49	0.48
1:A:171:ASN:C	1:A:173:GLU:H	2.22	0.48
1:A:380:TYR:CE2	1:A:382:LYS:HA	2.48	0.48
1:A:464:LYS:HG3	1:A:465:PRO:HD2	1.95	0.48
1:D:339:ASN:CG	1:D:340:PRO:HD2	2.38	0.48
1:C:449:LEU:CD2	1:C:472:PRO:HG2	2.44	0.48
1:B:223:MET:HE3	1:B:224:LYS:H	1.78	0.48
1:A:127:HIS:O	1:A:128:LEU:HD23	2.14	0.48
1:D:135:ILE:HG22	1:D:192:ILE:HB	1.96	0.48
1:C:87:ARG:HB3	1:C:218:LEU:HD12	1.96	0.48
1:B:103:PRO:HG2	1:B:214:LEU:HD23	1.95	0.48
1:A:135:ILE:HG21	1:A:206:ILE:HD13	1.96	0.48
1:D:338:HIS:CE1	1:D:559:ARG:NH2	2.82	0.48
1:B:200:LYS:H	1:B:200:LYS:HD3	1.77	0.47
1:C:407:ILE:HG12	1:C:457:ILE:HD11	1.96	0.47
1:C:574:ILE:O	1:C:577:PRO:HD3	2.14	0.47
1:B:534:GLN:O	1:B:535:LEU:HD12	2.13	0.47
1:A:116:ILE:O	1:A:120:LYS:HB3	2.14	0.47
1:D:217:CYS:SG	1:D:221:LEU:CD1	3.02	0.47
1:C:416:GLU:N	1:C:424:THR:HG21	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:HG23	1:B:135:ILE:HG22	1.97	0.47
1:C:192:ILE:HG23	1:C:208:PRO:HB3	1.97	0.47
1:C:280:LEU:HD23	1:C:280:LEU:HA	1.58	0.47
1:B:465:PRO:HA	1:B:495:PHE:O	2.14	0.46
1:D:141:ARG:HB3	1:D:153:ASP:HB2	1.97	0.46
1:C:135:ILE:HG22	1:C:192:ILE:HB	1.98	0.46
1:C:406:GLU:HG2	1:C:457:ILE:HG12	1.97	0.46
1:A:230:THR:HA	1:A:233:ARG:HE	1.81	0.46
1:C:416:GLU:O	1:C:424:THR:HG21	2.16	0.46
1:C:555:LEU:HD22	1:C:560:ILE:HD11	1.97	0.46
1:C:541:THR:O	1:C:545:TYR:HD2	1.99	0.46
1:C:353:ASP:OD2	1:C:483:ARG:NH2	2.37	0.46
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.62	0.46
1:D:140:MET:HE3	1:D:140:MET:HB3	1.87	0.46
1:C:275:THR:HB	1:C:276:PRO:HD2	1.98	0.46
1:C:440:PRO:O	1:C:443:PRO:HG3	2.15	0.46
1:C:571:LYS:HD3	1:C:579:MET:HE1	1.98	0.46
1:B:491:ARG:HG3	1:B:505:TYR:HD2	1.80	0.46
1:C:280:LEU:HD23	1:C:301:LEU:CD2	2.46	0.45
1:D:117:GLU:HA	1:D:120:LYS:HD2	1.99	0.45
1:B:346:GLU:OE1	2:B:601:KAA:HB1	2.16	0.45
1:A:135:ILE:HG22	1:A:206:ILE:HD13	1.98	0.45
1:A:138:ARG:NH2	1:A:189:ILE:HD11	2.31	0.45
1:A:261:LEU:HD21	1:A:345:CYS:SG	2.56	0.45
1:D:276:PRO:HD3	1:C:576:PHE:HB2	1.98	0.45
1:D:252:VAL:HG22	1:C:271:PHE:CE1	2.52	0.45
1:A:335:ASP:OD1	1:A:338:HIS:HB2	2.17	0.45
1:B:424:THR:O	1:B:428:MET:HG3	2.17	0.45
1:B:478:LEU:HD23	1:B:514:GLN:OE1	2.17	0.45
1:A:147:GLN:OE1	1:A:150:ARG:NH2	2.50	0.45
1:A:424:THR:HA	1:A:427:LYS:HG3	1.97	0.45
1:A:492:LEU:O	1:A:492:LEU:HG	2.16	0.45
1:D:234:TYR:OH	1:D:572:ASP:OD1	2.28	0.45
1:C:135:ILE:HD12	1:C:135:ILE:HA	1.73	0.45
1:B:357:LEU:HD13	1:B:504:ALA:HB1	1.98	0.45
1:D:231:GLU:O	1:D:235:ARG:HG3	2.17	0.45
1:C:290:PHE:HB2	1:C:303:LEU:HD12	1.99	0.45
1:B:439:LEU:HA	1:B:440:PRO:HD3	1.40	0.45
1:D:189:ILE:HG12	1:D:215:SER:O	2.16	0.45
1:A:148:LYS:O	1:A:149:LEU:HD23	2.17	0.45
1:A:230:THR:HA	1:A:233:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:THR:HG22	1:C:446:ALA:H	1.80	0.45
1:A:339:ASN:CG	1:A:340:PRO:HD2	2.43	0.44
1:A:478:LEU:HD21	1:A:535:LEU:HD11	1.99	0.44
1:A:420:ASP:OD1	1:A:420:ASP:N	2.40	0.44
1:D:205:SER:OG	1:D:206:ILE:N	2.50	0.44
1:A:222:PRO:HG2	1:A:243:ILE:CD1	2.48	0.44
1:D:164:LEU:HD23	1:D:165:ALA:N	2.31	0.44
1:D:415:LEU:HA	1:D:415:LEU:HD23	1.57	0.44
1:B:192:ILE:HG23	1:B:211:THR:HG22	1.99	0.44
1:C:339:ASN:OD1	1:C:340:PRO:HD2	2.17	0.44
1:B:429:ILE:HD11	1:B:443:PRO:HB2	1.98	0.44
1:B:472:PRO:HD2	1:B:475:MET:SD	2.58	0.43
1:D:148:LYS:HD3	1:D:167:TYR:CD2	2.53	0.43
1:D:148:LYS:CB	1:D:167:TYR:HB2	2.44	0.43
1:C:194:GLY:HA3	1:C:207:PHE:O	2.18	0.43
1:D:149:LEU:HA	1:D:149:LEU:HD23	1.75	0.43
1:C:440:PRO:HB2	1:C:443:PRO:HA	2.00	0.43
1:D:138:ARG:NH2	1:C:546:GLY:O	2.49	0.43
1:D:358:ILE:HG21	1:D:400:LYS:HE2	2.00	0.43
1:C:354:TYR:OH	1:C:469:VAL:HG11	2.18	0.43
1:B:91:ILE:HD12	1:B:91:ILE:HG23	1.72	0.43
1:C:386:GLU:H	1:C:386:GLU:CD	2.26	0.43
1:C:404:VAL:HG13	1:C:405:GLU:H	1.82	0.43
1:D:399:PRO:HG2	1:D:466:PHE:HB2	2.00	0.43
1:D:105:LYS:HE3	1:C:351:TYR:O	2.19	0.43
1:A:252:VAL:HG12	1:A:256:LYS:HE2	2.01	0.43
1:D:460:LYS:HG2	1:D:461:TYR:CE2	2.54	0.43
1:C:439:LEU:HA	1:C:440:PRO:HD3	1.20	0.43
1:C:176:ASN:HB3	1:C:179:GLU:HB2	2.01	0.43
1:B:127:HIS:HD2	1:B:129:GLU:OE2	2.02	0.42
1:B:363:ASP:O	1:B:367:GLN:HG3	2.19	0.42
1:D:233:ARG:HA	1:D:240:ASP:HB2	2.00	0.42
1:B:200:LYS:HB2	1:B:200:LYS:HE2	1.88	0.42
1:B:415:LEU:HD11	1:B:428:MET:HG2	2.01	0.42
1:B:505:TYR:CZ	2:B:601:KAA:HE2	2.53	0.42
1:B:116:ILE:O	1:B:120:LYS:HB3	2.19	0.42
1:B:358:ILE:HD13	1:B:492:LEU:HD13	2.01	0.42
1:B:401:VAL:HG21	1:B:460:LYS:HD3	2.02	0.42
1:B:413:THR:O	1:B:414:ILE:HD13	2.19	0.42
1:D:191:GLY:O	1:D:211:THR:HA	2.19	0.42
1:A:112:ILE:HG13	1:A:135:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:CB	1:A:150:ARG:HD3	2.50	0.42
1:A:339:ASN:OD1	1:A:340:PRO:HD2	2.19	0.42
1:C:422:ASN:OD1	1:C:422:ASN:N	2.52	0.42
1:D:189:ILE:CG1	1:D:215:SER:HB3	2.49	0.42
1:B:181:TYR:OH	1:B:211:THR:HG23	2.19	0.42
1:A:155:VAL:HA	1:A:159:GLU:O	2.20	0.42
1:A:162:GLN:O	1:A:205:SER:HA	2.18	0.42
1:C:417:GLN:HA	1:C:418:PRO:C	2.44	0.42
1:A:171:ASN:C	1:A:173:GLU:N	2.78	0.41
1:C:390:ILE:HD11	1:C:497:CYS:SG	2.60	0.41
1:B:307:THR:O	1:B:310:PRO:HD2	2.20	0.41
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.54	0.41
1:D:213:LEU:HD11	1:D:216:ALA:HA	2.03	0.41
1:D:380:TYR:HE1	1:D:563:PHE:HA	1.84	0.41
1:C:330:ARG:NH2	2:C:601:KAA:O2S	2.53	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.93	0.41
1:B:330:ARG:NH1	2:B:601:KAA:O1S	2.53	0.41
1:C:453:ALA:HA	1:C:457:ILE:CD1	2.50	0.41
1:A:508:LEU:C	1:A:508:LEU:HD23	2.45	0.41
1:D:373:PHE:O	1:D:375:THR:HG22	2.19	0.41
1:C:412:ASN:ND2	1:C:412:ASN:C	2.76	0.41
1:C:502:LEU:C	1:C:502:LEU:HD12	2.45	0.41
1:D:227:LEU:HA	1:D:227:LEU:HD23	1.62	0.41
1:D:168:SER:H	1:D:168:SER:HG	1.56	0.41
1:D:238:TYR:CD1	1:D:239:LEU:HG	2.55	0.41
1:D:439:LEU:HA	1:D:440:PRO:HD2	1.11	0.41
1:C:110:ILE:HD13	1:C:110:ILE:HG21	1.90	0.41
1:A:375:THR:OG1	1:A:376:TYR:N	2.53	0.41
1:D:245:GLU:H	1:D:245:GLU:HG2	1.68	0.41
1:D:534:GLN:C	1:D:535:LEU:HD23	2.46	0.41
1:D:543:LEU:HD23	1:D:543:LEU:HA	1.89	0.41
1:C:491:ARG:HG3	1:C:505:TYR:HD2	1.85	0.41
1:B:308:GLU:OE1	2:B:601:KAA:NZ	2.54	0.41
1:C:449:LEU:HB3	1:C:475:MET:CE	2.51	0.41
1:C:472:PRO:HD2	1:C:475:MET:SD	2.61	0.41
1:B:504:ALA:HB2	1:B:553:LEU:HG	2.03	0.40
1:A:252:VAL:CG1	1:A:256:LYS:HE2	2.50	0.40
1:A:474:ILE:O	1:A:474:ILE:HG13	2.21	0.40
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.91	0.40
1:C:346:GLU:CD	2:C:601:KAA:HN1	2.29	0.40
1:B:492:LEU:O	1:B:492:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:O	1:A:101:PRO:HD3	2.21	0.40
1:A:470:GLU:HA	1:A:489:THR:O	2.21	0.40
1:C:319:ILE:HG22	1:C:322:VAL:HB	2.03	0.40
1:B:416:GLU:N	1:B:424:THR:HG21	2.34	0.40
1:D:384:GLY:HA2	1:D:385:PRO:HD3	1.80	0.40
1:C:404:VAL:HG13	1:C:405:GLU:N	2.36	0.40
1:C:537:SER:O	1:C:541:THR:HG23	2.21	0.40
1:B:325:ILE:HG12	1:B:345:CYS:HB2	2.04	0.40
1:D:219:HIS:NE2	1:C:544:GLU:OE1	2.48	0.40
1:D:290:PHE:HB2	1:D:303:LEU:HG	2.03	0.40
1:D:338:HIS:HE1	1:D:559:ARG:HH22	1.69	0.40
1:D:380:TYR:CE2	1:D:382:LYS:HA	2.56	0.40

There are no symmetry-related clashes.

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	480/507 (95%)	462 (96%)	17 (4%)	1 (0%)	43	63
1	B	483/507 (95%)	466 (96%)	17 (4%)	0	100	100
1	C	471/507 (93%)	454 (96%)	16 (3%)	1 (0%)	43	63
1	D	477/507 (94%)	453 (95%)	23 (5%)	1 (0%)	43	63
All	All	1911/2028 (94%)	1835 (96%)	73 (4%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	440	PRO
1	C	442	PRO
1	A	442	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	424/457 (93%)	422 (100%)	2 (0%)	81	92
1	B	430/457 (94%)	429 (100%)	1 (0%)	87	95
1	C	401/457 (88%)	400 (100%)	1 (0%)	87	95
1	D	384/457 (84%)	378 (98%)	6 (2%)	55	79
All	All	1639/1828 (90%)	1629 (99%)	10 (1%)	78	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	437	ILE
1	A	227	LEU
1	A	330	ARG
1	D	164	LEU
1	D	223	MET
1	D	390	ILE
1	D	391	GLU
1	D	415	LEU
1	D	420	ASP
1	C	330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	263	ASN
1	B	387	ASN
1	A	176	ASN
1	A	451	GLN
1	A	462	ASN
1	D	387	ASN
1	D	417	GLN
1	D	451	GLN
1	D	503	ASN

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Mol	Chain	Res	Type
1	C	387	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](#)

4 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	KAA	A	601	-	34,34,34	1.26	3 (8%)	46,49,49	1.19	4 (8%)
2	KAA	D	601	-	34,34,34	1.06	2 (5%)	46,49,49	0.99	3 (6%)
2	KAA	C	601	-	34,34,34	1.35	2 (5%)	46,49,49	1.01	1 (2%)
2	KAA	B	601	-	34,34,34	1.37	4 (11%)	46,49,49	1.09	4 (8%)

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	KAA	A	601	-	-	4/23/40/40	0/3/3/3
2	KAA	D	601	-	-	3/23/40/40	0/3/3/3
2	KAA	C	601	-	-	6/23/40/40	0/3/3/3
2	KAA	B	601	-	-	5/23/40/40	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	KAA	S1-N8	-4.53	1.52	1.59
2	C	601	KAA	C-N8	-4.41	1.29	1.37
2	B	601	KAA	C-N8	-3.27	1.31	1.37
2	A	601	KAA	S1-N8	-3.24	1.54	1.59
2	D	601	KAA	S1-N8	-3.21	1.54	1.59
2	A	601	KAA	C-N8	-3.18	1.31	1.37
2	B	601	KAA	O5'-S1	-3.03	1.53	1.60
2	D	601	KAA	C-N8	-2.86	1.32	1.37
2	B	601	KAA	S1-N8	-2.20	1.56	1.59
2	A	601	KAA	O5'-S1	-2.14	1.55	1.60
2	B	601	KAA	CA-N	-2.07	1.38	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	KAA	O5'-S1-O2S	-5.04	90.24	105.48
2	C	601	KAA	CB-CA-N	-4.70	97.88	110.12
2	D	601	KAA	CB-CA-N	-3.95	99.83	110.12
2	B	601	KAA	O-C-N8	-3.40	116.80	122.98
2	A	601	KAA	O5'-S1-O1S	3.37	115.67	105.48
2	B	601	KAA	O5'-S1-O2S	-3.34	95.39	105.48
2	D	601	KAA	C-N8-S1	-2.59	114.61	124.07
2	A	601	KAA	C-N8-S1	-2.52	114.84	124.07
2	B	601	KAA	CG-CB-CA	-2.37	105.57	113.22
2	D	601	KAA	O5'-S1-O2S	2.23	112.24	105.48
2	B	601	KAA	O2'-C2'-C1'	-2.21	102.48	110.10
2	A	601	KAA	CB-CA-N	-2.09	104.68	110.12

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	KAA	O4'-C4'-C5'-O5'

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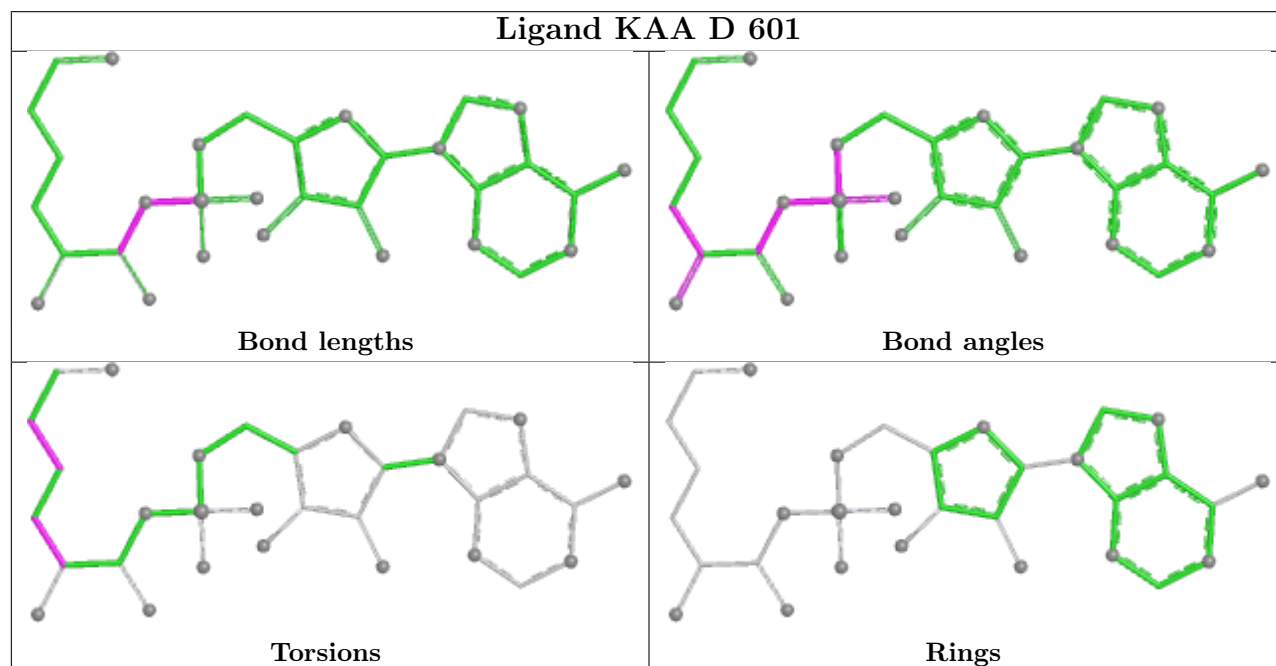
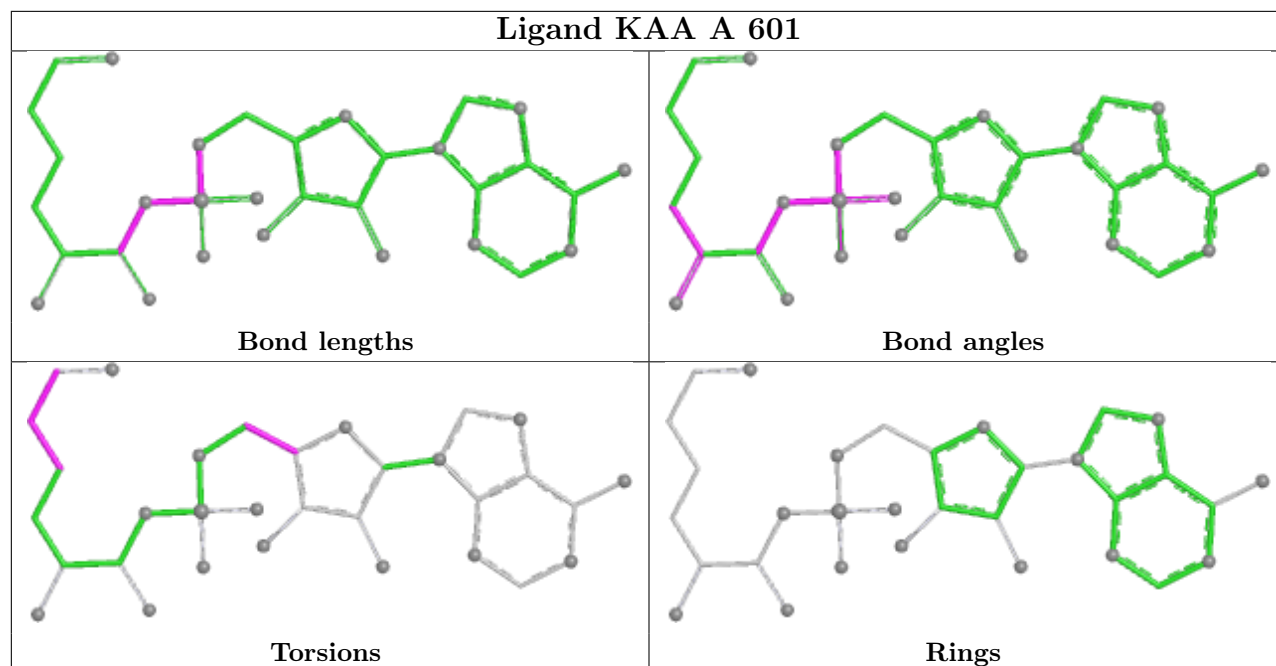
Mol	Chain	Res	Type	Atoms
2	B	601	KAA	C3'-C4'-C5'-O5'
2	A	601	KAA	O4'-C4'-C5'-O5'
2	A	601	KAA	C3'-C4'-C5'-O5'
2	D	601	KAA	N-CA-CB-CG
2	D	601	KAA	C-CA-CB-CG
2	C	601	KAA	C3'-C4'-C5'-O5'
2	B	601	KAA	C-CA-CB-CG
2	B	601	KAA	CG-CD-CE-NZ
2	C	601	KAA	C-N8-S1-O1S
2	B	601	KAA	N-CA-CB-CG
2	C	601	KAA	CG-CD-CE-NZ
2	D	601	KAA	CE-CD-CG-CB
2	C	601	KAA	CE-CD-CG-CB
2	C	601	KAA	CA-CB-CG-CD
2	A	601	KAA	CE-CD-CG-CB
2	A	601	KAA	CG-CD-CE-NZ
2	C	601	KAA	O4'-C4'-C5'-O5'

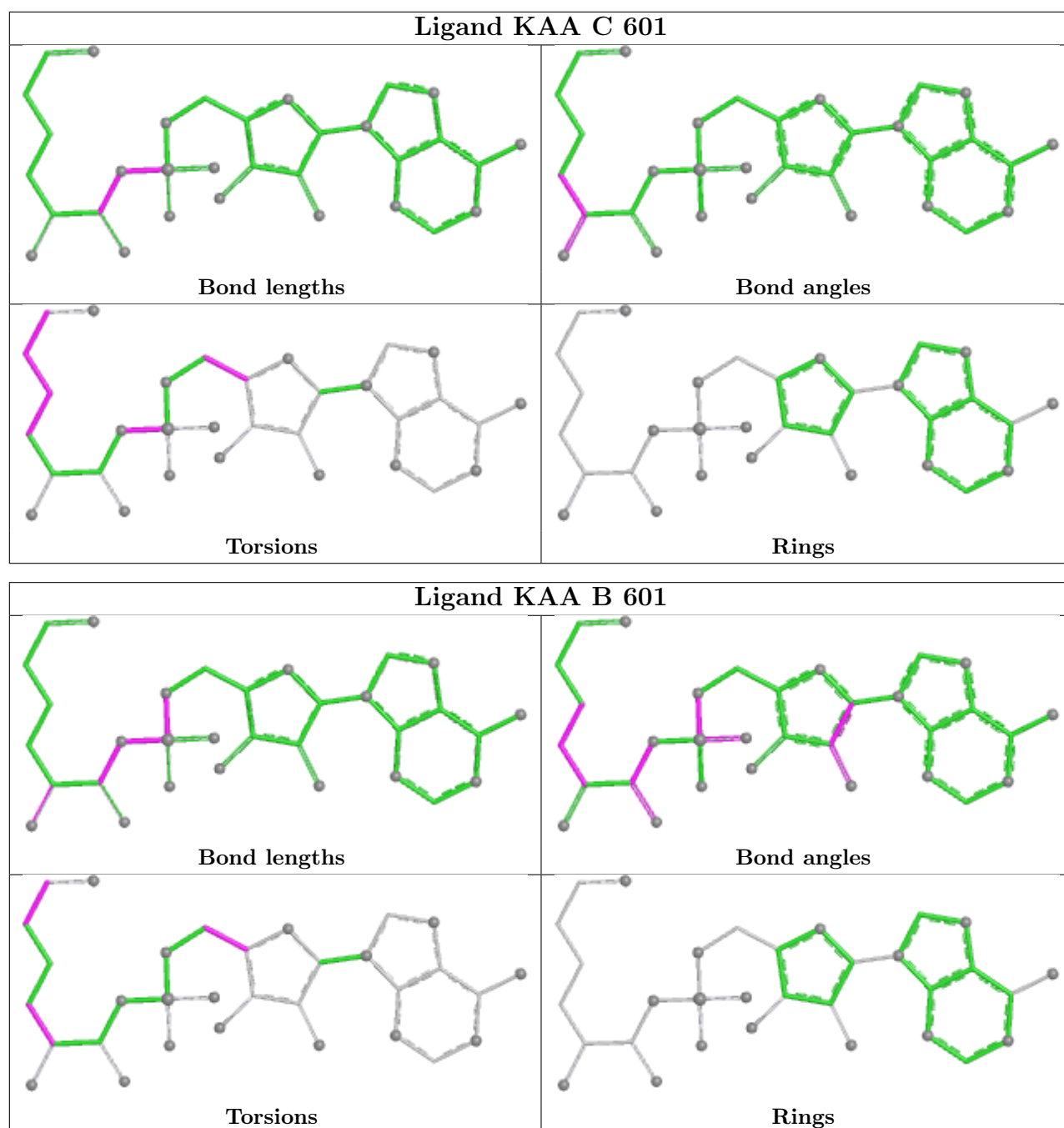
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	KAA	3	0
2	C	601	KAA	3	0
2	B	601	KAA	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	486/507 (95%)	0.29	20 (4%) 41 37	59, 81, 119, 141	1 (0%)
1	B	487/507 (96%)	0.30	16 (3%) 49 45	61, 80, 115, 162	0
1	C	479/507 (94%)	0.48	21 (4%) 39 34	65, 87, 133, 177	0
1	D	483/507 (95%)	0.83	64 (13%) 7 6	64, 97, 142, 172	0
All	All	1935/2028 (95%)	0.48	121 (6%) 26 23	59, 85, 132, 177	1 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	THR	7.3
1	C	282	ALA	7.0
1	A	285	ALA	6.7
1	B	282	ALA	6.0
1	D	191	GLY	5.8
1	A	80	PRO	5.3
1	C	80	PRO	5.1
1	D	80	PRO	5.0
1	B	80	PRO	4.8
1	D	81	ARG	4.7
1	D	286	ASN	4.5
1	D	281	ILE	4.4
1	A	334	ILE	4.2
1	D	163	VAL	4.2
1	D	193	VAL	4.2
1	A	282	ALA	4.2
1	D	192	ILE	4.1
1	D	169	PHE	4.1
1	D	518	PHE	4.0
1	B	284	GLY	3.9
1	B	518	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	151	PHE	3.8
1	D	82	LEU	3.7
1	A	441	ASN	3.7
1	C	514	GLN	3.6
1	C	534	GLN	3.6
1	A	581	PRO	3.5
1	D	212	ILE	3.5
1	A	348	TYR	3.4
1	A	514	GLN	3.3
1	A	284	GLY	3.3
1	C	332	GLU	3.2
1	D	410	VAL	3.2
1	C	287	ALA	3.2
1	D	180	CYS	3.2
1	B	147	GLN	3.1
1	D	152	PHE	3.1
1	D	129	GLU	3.0
1	D	145	SER	3.0
1	D	424	THR	3.0
1	D	194	GLY	2.9
1	D	225	TYR	2.9
1	D	288	ARG	2.9
1	A	354	TYR	2.9
1	C	535	LEU	2.8
1	B	340	PRO	2.8
1	D	190	VAL	2.7
1	D	181	TYR	2.7
1	C	419	PHE	2.7
1	A	442	PRO	2.7
1	B	285	ALA	2.7
1	B	283	GLY	2.6
1	C	518	PHE	2.6
1	A	518	PHE	2.6
1	D	177	PHE	2.6
1	D	128	LEU	2.6
1	D	230	THR	2.6
1	D	456	PHE	2.5
1	A	534	GLN	2.5
1	D	178	ALA	2.5
1	D	143	SER	2.5
1	D	481	TYR	2.5
1	A	283	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	137	GLY	2.4
1	B	135	ILE	2.4
1	D	139	ILE	2.4
1	C	516	GLU	2.4
1	D	187	GLY	2.4
1	D	214	LEU	2.4
1	D	150	ARG	2.4
1	C	338	HIS	2.4
1	D	203	GLU	2.4
1	C	421	SER	2.3
1	B	387	ASN	2.3
1	C	81	ARG	2.3
1	D	132	ILE	2.3
1	D	301	LEU	2.3
1	A	224	LYS	2.3
1	B	81	ARG	2.3
1	D	421	SER	2.3
1	B	192	ILE	2.3
1	D	200	LYS	2.3
1	B	354	TYR	2.3
1	D	146	GLY	2.3
1	A	142	VAL	2.3
1	D	430	ASN	2.2
1	C	297	LEU	2.2
1	A	339	ASN	2.2
1	D	199	SER	2.2
1	D	182	ASP	2.2
1	C	296	ASP	2.2
1	B	337	THR	2.2
1	B	415	LEU	2.2
1	D	201	LYS	2.2
1	D	444	THR	2.2
1	D	142	VAL	2.1
1	D	221	LEU	2.1
1	D	354	TYR	2.1
1	D	416	GLU	2.1
1	D	93	ASP	2.1
1	D	211	THR	2.1
1	D	340	PRO	2.1
1	C	299	LEU	2.1
1	D	334	ILE	2.1
1	C	281	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	464	LYS	2.1
1	B	143	SER	2.1
1	D	333	GLY	2.1
1	D	161	ILE	2.1
1	D	437	ILE	2.1
1	A	225	TYR	2.1
1	A	144	ALA	2.0
1	C	452	LEU	2.0
1	A	426	GLU	2.0
1	D	91	ILE	2.0
1	D	135	ILE	2.0
1	D	388	GLN	2.0
1	D	189	ILE	2.0
1	D	337	THR	2.0
1	C	230	THR	2.0
1	C	277	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

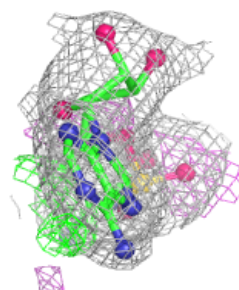
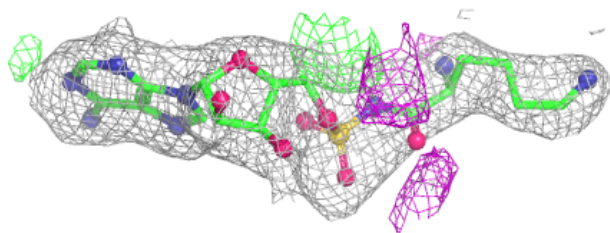
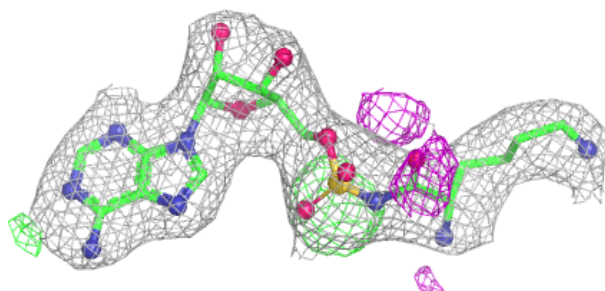
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KAA	B	601	32/32	0.91	0.11	61,63,88,97	0
2	KAA	D	601	32/32	0.91	0.12	62,74,85,89	32
2	KAA	A	601	32/32	0.92	0.11	63,65,96,115	0
2	KAA	C	601	32/32	0.92	0.11	70,83,93,99	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

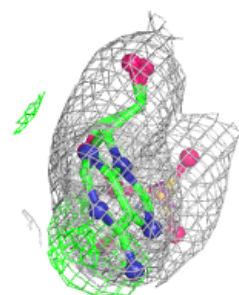
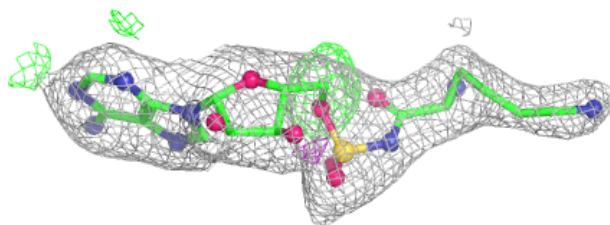
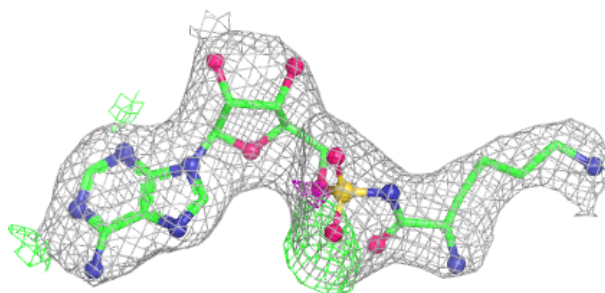
Electron density around KAA B 601:

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



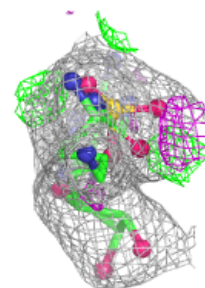
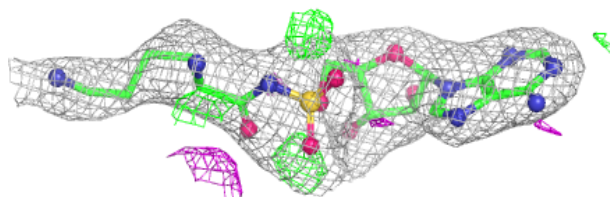
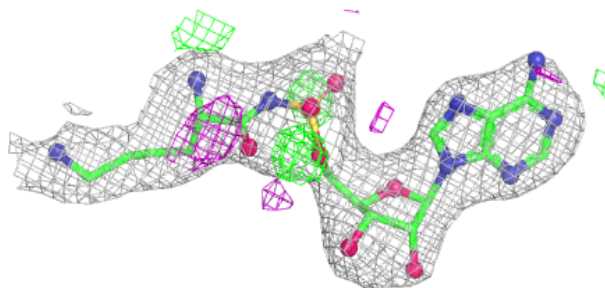
Electron density around KAA D 601:

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

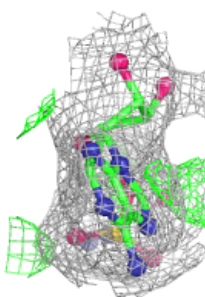
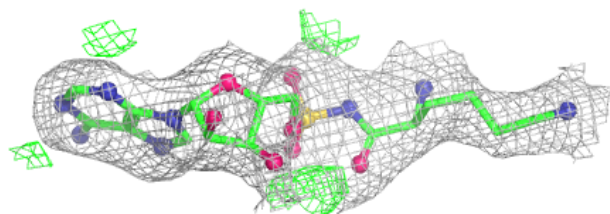
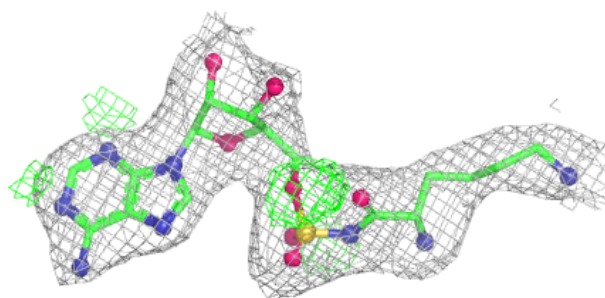


Electron density around KAA A 601:

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

**Electron density around KAA C 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.