



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:46 AM UTC

PDB ID : 8BIQ / pdb_00008biq
Title : Crystal structure of acyl-CoA synthetase from *Metallosphaera sedula* in complex with acetyl-AMP
Authors : Capra, N.; Thunnissen, A.M.W.H.; Janssen, D.B.
Deposited on : 2022-11-02
Resolution : 2.80 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

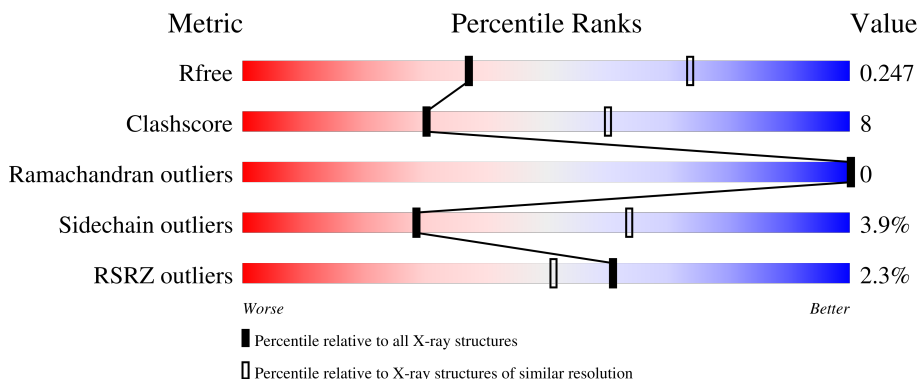
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

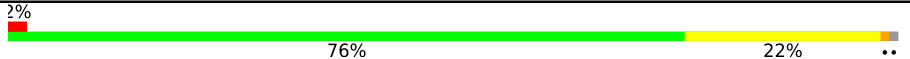
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	570	 2% 76% 22% ..
1	B	570	 2% 74% 21% . .
1	C	570	 2% 77% 19% . .
1	D	570	 2% 74% 22% . . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18127 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 4-hydroxybutyrate--CoA ligase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	561	Total	C	N	O	S	0	0	0
			4519	2905	764	837	13			
1	A	562	Total	C	N	O	S	0	0	0
			4526	2909	765	839	13			
1	B	561	Total	C	N	O	S	0	0	0
			4519	2905	764	837	13			
1	C	554	Total	C	N	O	S	0	0	0
			4468	2872	755	828	13			

There are 28 discrepancies between the modelled and reference sequences:

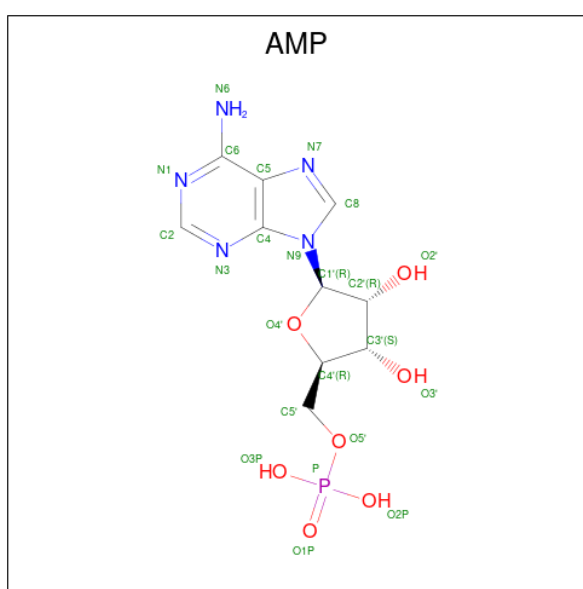
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A4YDT1
D	2	HIS	-	expression tag	UNP A4YDT1
D	3	HIS	-	expression tag	UNP A4YDT1
D	4	HIS	-	expression tag	UNP A4YDT1
D	5	HIS	-	expression tag	UNP A4YDT1
D	6	HIS	-	expression tag	UNP A4YDT1
D	7	HIS	-	expression tag	UNP A4YDT1
A	1	MET	-	initiating methionine	UNP A4YDT1
A	2	HIS	-	expression tag	UNP A4YDT1
A	3	HIS	-	expression tag	UNP A4YDT1
A	4	HIS	-	expression tag	UNP A4YDT1
A	5	HIS	-	expression tag	UNP A4YDT1
A	6	HIS	-	expression tag	UNP A4YDT1
A	7	HIS	-	expression tag	UNP A4YDT1
B	1	MET	-	initiating methionine	UNP A4YDT1
B	2	HIS	-	expression tag	UNP A4YDT1
B	3	HIS	-	expression tag	UNP A4YDT1
B	4	HIS	-	expression tag	UNP A4YDT1
B	5	HIS	-	expression tag	UNP A4YDT1
B	6	HIS	-	expression tag	UNP A4YDT1
B	7	HIS	-	expression tag	UNP A4YDT1

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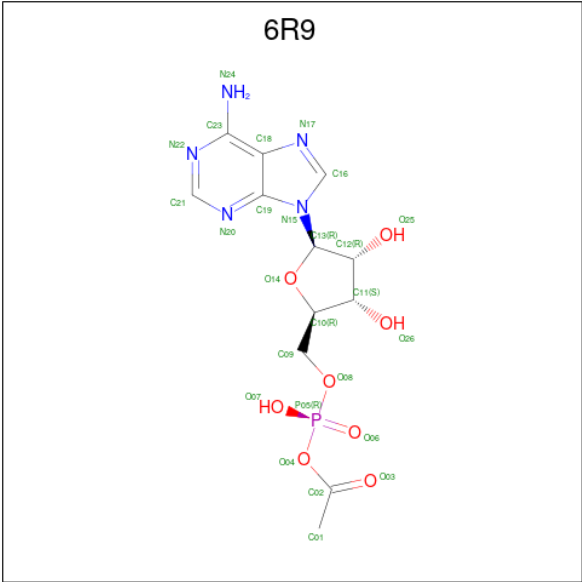
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A4YDT1
C	2	HIS	-	expression tag	UNP A4YDT1
C	3	HIS	-	expression tag	UNP A4YDT1
C	4	HIS	-	expression tag	UNP A4YDT1
C	5	HIS	-	expression tag	UNP A4YDT1
C	6	HIS	-	expression tag	UNP A4YDT1
C	7	HIS	-	expression tag	UNP A4YDT1

- Molecule 2 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
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] ethanoate (CCD ID: 6R9) (formula: $C_{12}H_{16}N_5O_8P$) (labeled as "Ligand of Interest" by depositor).

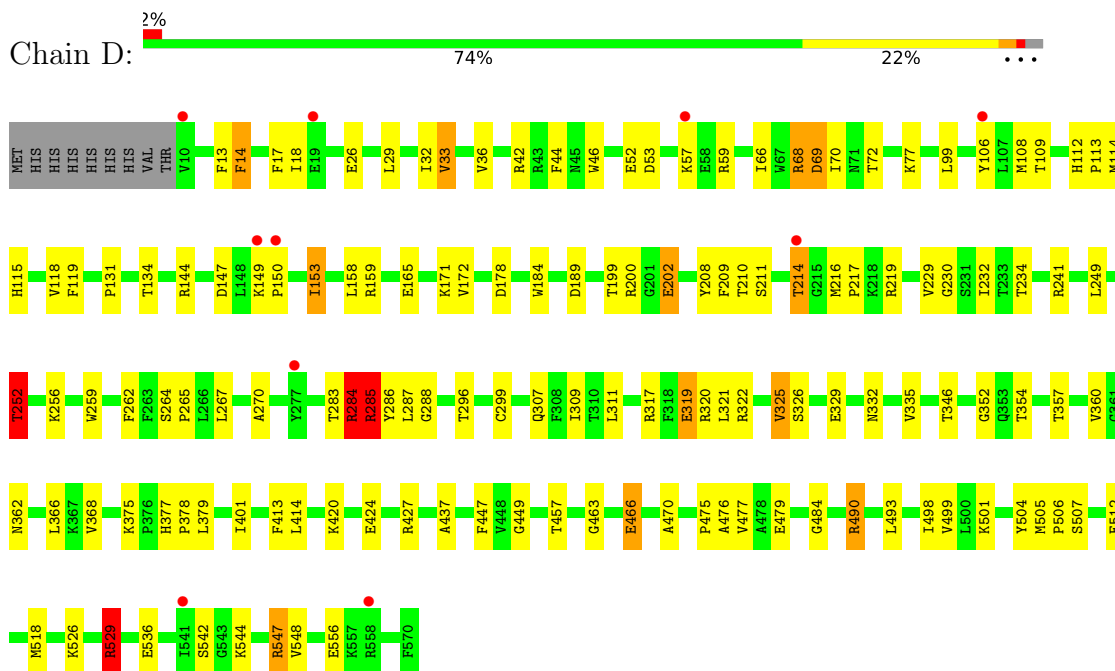


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			26	12	5	8	1		

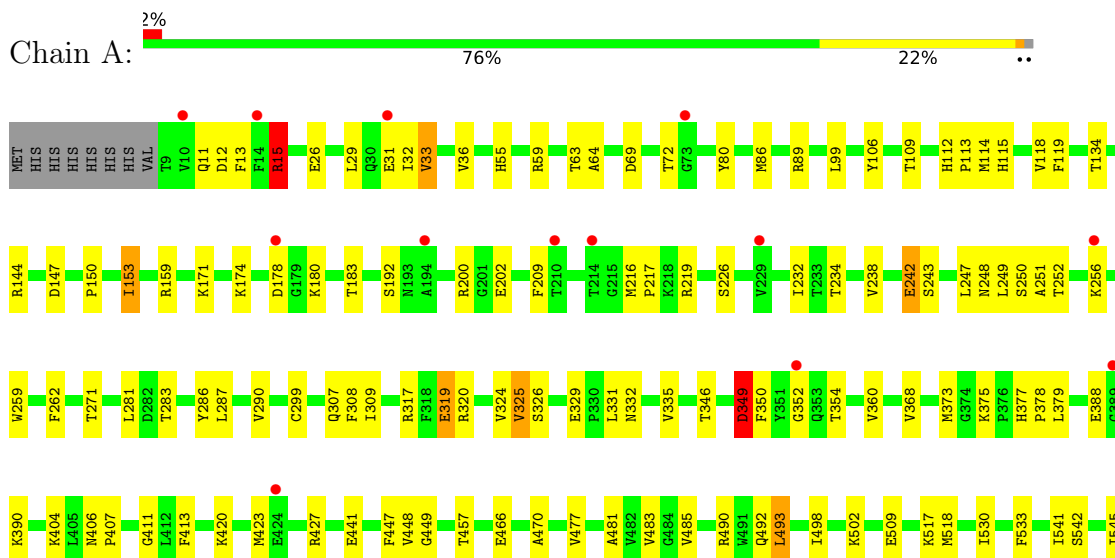
3 Residue-property plots

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: 4-hydroxybutyrate--CoA ligase 1

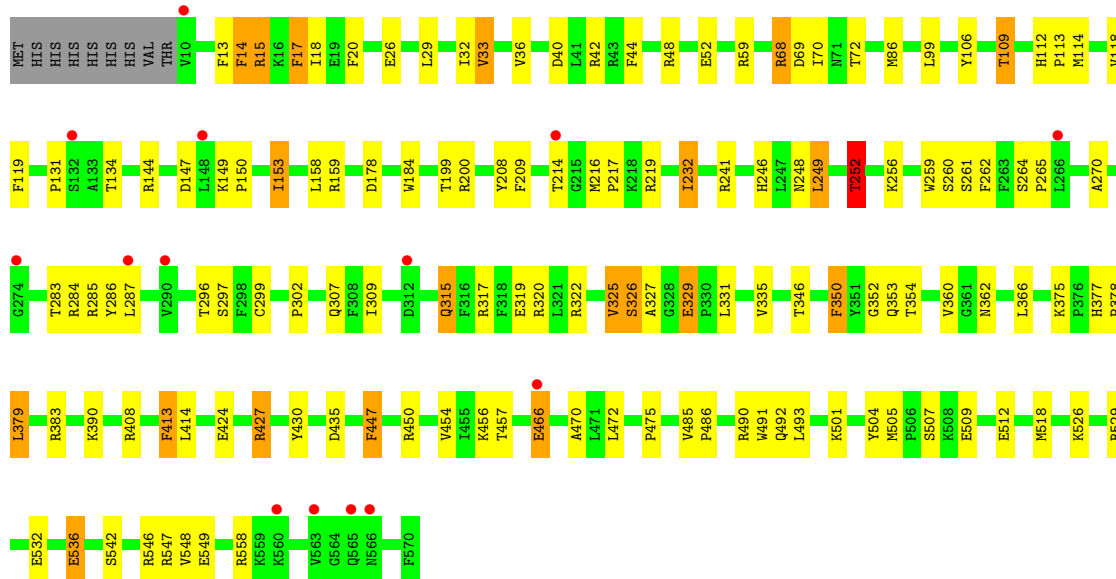
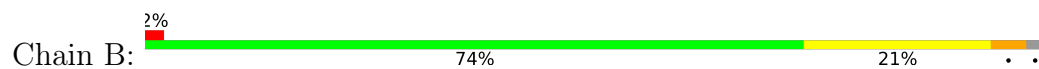


• Molecule 1: 4-hydroxybutyrate--CoA ligase 1

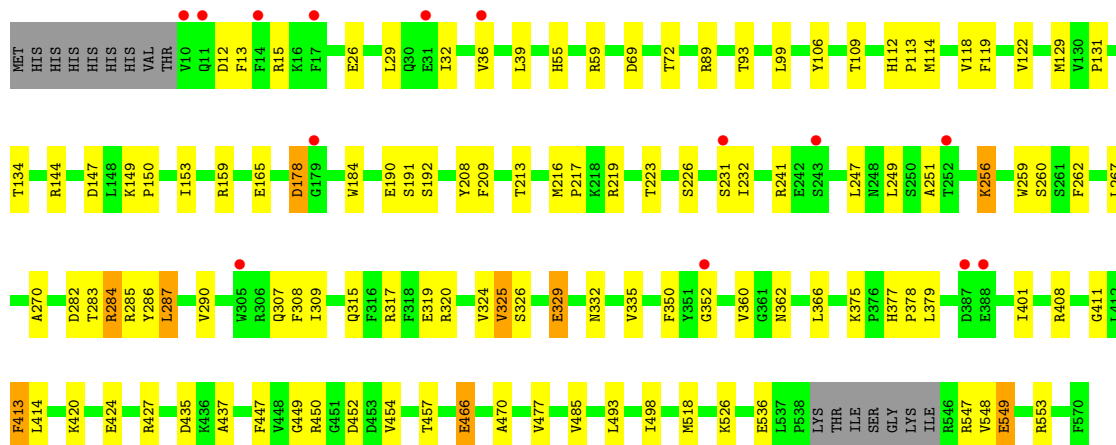
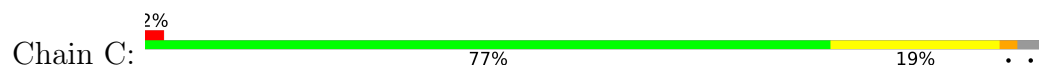




• Molecule 1: 4-hydroxybutyrate--CoA ligase 1



• Molecule 1: 4-hydroxybutyrate--CoA ligase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.86Å 88.29Å 131.21Å 90.00° 92.97° 90.00°	Depositor
Resolution (Å)	66.48 – 2.80 66.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.48-2.80) 99.7 (66.48-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.235 , 0.273 0.238 , 0.247	Depositor DCC
R_{free} test set	2943 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	1.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18127	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.60% 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: AMP, 6R9

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	0.74	0/4631	1.36	17/6257 (0.3%)
1	B	0.71	0/4624	1.33	20/6247 (0.3%)
1	C	0.68	0/4572	1.29	11/6177 (0.2%)
1	D	0.69	0/4624	1.29	18/6247 (0.3%)
All	All	0.71	0/18451	1.32	66/24928 (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	4
1	B	0	6
1	C	0	4
1	D	0	7
All	All	0	21

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	PHE	CA-CB-CG	8.70	122.50	113.80
1	A	180	LYS	CB-CA-C	-8.13	95.77	109.50
1	D	165	GLU	CB-CG-CD	7.54	125.42	112.60
1	C	149	LYS	CB-CG-CD	7.40	128.31	111.30
1	A	15	ARG	CB-CA-C	7.38	123.40	110.85
1	B	466	GLU	N-CA-CB	-7.13	99.64	110.12
1	A	349	ASP	CA-CB-CG	7.12	119.72	112.60
1	B	252	THR	CA-CB-OG1	-6.93	99.21	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	299	CYS	CB-CA-C	-6.80	98.65	109.80
1	B	15	ARG	CB-CA-C	6.72	122.27	110.85
1	A	319	GLU	CB-CG-CD	6.70	123.98	112.60
1	C	466	GLU	N-CA-CB	-6.69	100.29	110.12
1	A	171	LYS	CB-CA-C	-6.51	100.78	110.16
1	B	322	ARG	CG-CD-NE	-6.50	97.70	112.00
1	D	466	GLU	N-CA-CB	-6.44	100.65	110.12
1	D	202	GLU	CB-CG-CD	6.42	123.52	112.60
1	C	15	ARG	CB-CA-C	6.39	121.72	110.85
1	C	178	ASP	CA-CB-CG	6.39	118.99	112.60
1	B	536	GLU	CB-CG-CD	6.35	123.39	112.60
1	D	457	THR	CA-CB-OG1	-6.16	100.36	109.60
1	D	319	GLU	CB-CG-CD	6.13	123.02	112.60
1	D	214	THR	CA-CB-OG1	-6.10	100.45	109.60
1	D	252	THR	OG1-CB-CG2	6.10	121.50	109.30
1	B	178	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	447	PHE	CB-CA-C	-6.10	99.23	109.65
1	D	556	GLU	CB-CG-CD	6.07	122.93	112.60
1	B	325	VAL	N-CA-CB	-6.07	100.57	111.92
1	A	325	VAL	N-CA-CB	-6.06	101.16	112.36
1	D	178	ASP	CA-CB-CG	6.05	118.65	112.60
1	D	512	GLU	CB-CA-C	-5.91	101.60	110.88
1	D	234	THR	CA-CB-OG1	5.89	118.43	109.60
1	B	149	LYS	CB-CG-CD	5.86	124.78	111.30
1	B	512	GLU	CB-CA-C	-5.72	101.90	110.88
1	D	17	PHE	CA-CB-CG	-5.58	108.22	113.80
1	C	319	GLU	CB-CG-CD	5.57	122.07	112.60
1	B	52	GLU	CB-CG-CD	5.54	122.03	112.60
1	D	322	ARG	N-CA-CB	-5.51	102.66	110.81
1	B	532	GLU	CB-CG-CD	5.47	121.90	112.60
1	C	450	ARG	N-CA-CB	-5.47	101.80	110.06
1	B	315	GLN	CB-CA-C	-5.47	98.88	110.31
1	B	17	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	31	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	354	THR	OG1-CB-CG2	-5.38	98.53	109.30
1	A	502	LYS	CB-CA-C	5.38	118.29	109.90
1	C	213	THR	CB-CA-C	5.32	119.72	110.79
1	A	556	GLU	N-CA-CB	5.30	118.49	110.28
1	B	509	GLU	CB-CG-CD	5.30	121.61	112.60
1	D	69	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	325	VAL	N-CA-CB	-5.27	102.06	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ASP	CB-CA-C	-5.20	101.00	110.63
1	A	171	LYS	N-CA-CB	5.20	117.73	109.51
1	A	466	GLU	N-CA-CB	-5.18	102.50	110.12
1	C	165	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	349	ASP	CB-CA-C	5.16	118.95	109.46
1	D	171	LYS	CB-CA-C	-5.16	102.53	110.26
1	B	529	ARG	CG-CD-NE	-5.15	100.66	112.00
1	B	354	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	14	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	214	THR	CA-CB-OG1	-5.09	101.97	109.60
1	D	529	ARG	NE-CZ-NH1	-5.05	116.44	121.50
1	D	189	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	223	THR	CA-CB-OG1	5.04	117.16	109.60
1	C	329	GLU	CB-CA-C	-5.02	104.63	110.76
1	D	14	PHE	CA-CB-CG	-5.01	108.79	113.80
1	A	509	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain
1	A	251	ALA	Peptide
1	A	427	ARG	Sidechain
1	A	490	ARG	Sidechain
1	B	15	ARG	Sidechain
1	B	427	ARG	Sidechain
1	B	48	ARG	Sidechain
1	B	490	ARG	Sidechain
1	B	59	ARG	Sidechain
1	B	68	ARG	Sidechain
1	C	251	ALA	Peptide
1	C	284	ARG	Sidechain
1	C	320	ARG	Sidechain
1	C	547	ARG	Sidechain
1	D	284	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	490	ARG	Sidechain
1	D	529	ARG	Sidechain
1	D	547	ARG	Sidechain
1	D	59	ARG	Sidechain
1	D	68	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	4526	0	4542	83	0
1	B	4519	0	4535	75	0
1	C	4468	0	4471	63	0
1	D	4519	0	4535	95	0
2	A	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	0	0
3	B	26	0	0	0	0
All	All	18127	0	18119	306	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 8.

All (306) 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:283:THR:HG21	1:C:307:GLN:HB3	1.53	0.87
1:A:457:THR:HG22	1:A:492:GLN:O	1.77	0.85
1:A:483:VAL:HG12	1:A:547:ARG:HD3	1.60	0.83
1:B:547:ARG:HG3	1:B:547:ARG:HH11	1.41	0.83
1:A:547:ARG:HH11	1:A:547:ARG:HG3	1.43	0.82
1:A:256:LYS:NZ	1:A:259:TRP:CZ3	2.47	0.82
1:D:414:LEU:HB3	1:A:541:ILE:CG2	2.11	0.81
1:D:547:ARG:HG3	1:D:547:ARG:HH11	1.46	0.80
1:B:362:ASN:HA	1:B:366:LEU:HD23	1.65	0.79
1:A:283:THR:HG21	1:A:307:GLN:HB3	1.64	0.77
1:A:320:ARG:HG3	1:A:320:ARG:HH11	1.49	0.77
1:D:229:VAL:O	1:D:232:ILE:HG12	1.85	0.76
1:D:317:ARG:HD2	1:D:319:GLU:OE2	1.87	0.75
1:D:414:LEU:HB3	1:A:541:ILE:HG21	1.69	0.75
1:D:362:ASN:HA	1:D:366:LEU:HD23	1.68	0.74
1:D:53:ASP:HA	1:D:57:LYS:HD2	1.69	0.74
1:D:542:SER:HB2	1:A:390:LYS:HE2	1.74	0.70
1:D:14:PHE:HE1	1:D:232:ILE:HD11	1.57	0.68
1:D:108:MET:HE3	1:D:159:ARG:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:ARG:HG3	1:B:547:ARG:NH1	2.07	0.67
1:B:14:PHE:O	1:B:18:ILE:HG13	1.96	0.66
1:B:504:TYR:O	1:B:505:MET:HE2	1.96	0.65
1:D:379:LEU:HD23	1:D:379:LEU:O	1.95	0.65
1:D:504:TYR:O	1:D:505:MET:HE2	1.97	0.65
1:D:70:ILE:CG2	1:D:285:ARG:HG3	2.27	0.65
1:D:52:GLU:O	1:D:57:LYS:HG3	1.97	0.64
1:A:325:VAL:CG1	1:A:350:PHE:HE1	2.09	0.64
1:B:109:THR:O	1:B:252:THR:HG21	1.98	0.64
1:D:424:GLU:O	1:D:427:ARG:NH1	2.31	0.63
1:A:281:LEU:HD21	1:A:283:THR:HG22	1.80	0.63
1:D:53:ASP:OD1	1:D:57:LYS:NZ	2.31	0.63
1:D:210:THR:HG21	1:D:354:THR:HG21	1.79	0.63
1:C:379:LEU:O	1:C:379:LEU:HD23	1.98	0.62
1:D:134:THR:HB	1:D:159:ARG:NE	2.15	0.62
1:B:283:THR:HG21	1:B:307:GLN:HB3	1.81	0.62
1:C:134:THR:HB	1:C:159:ARG:NE	2.15	0.62
1:D:477:VAL:HG13	1:D:498:ILE:HG23	1.82	0.61
1:C:466:GLU:OE2	1:C:526:LYS:NZ	2.33	0.61
1:C:424:GLU:O	1:C:427:ARG:NH1	2.33	0.61
1:D:542:SER:HB2	1:A:390:LYS:CE	2.29	0.61
1:C:259:TRP:HH2	1:C:352:GLY:HA3	1.66	0.60
1:C:362:ASN:HA	1:C:366:LEU:HD23	1.82	0.60
1:C:325:VAL:CG1	1:C:350:PHE:HE1	2.14	0.60
1:A:477:VAL:HG13	1:A:498:ILE:HG23	1.84	0.60
1:B:134:THR:HB	1:B:159:ARG:NE	2.16	0.60
1:D:70:ILE:O	1:D:70:ILE:HG22	2.01	0.60
1:C:32:ILE:O	1:C:36:VAL:HG23	2.02	0.60
1:D:547:ARG:HG3	1:D:547:ARG:NH1	2.15	0.60
1:A:325:VAL:CG1	1:A:350:PHE:CE1	2.85	0.59
1:D:70:ILE:HG21	1:D:285:ARG:HG3	1.84	0.59
1:C:249:LEU:HD13	1:C:286:TYR:CZ	2.37	0.59
1:A:32:ILE:O	1:A:36:VAL:HG23	2.03	0.59
1:A:248:ASN:ND2	1:A:250:SER:HB3	2.18	0.59
1:A:249:LEU:HD13	1:A:286:TYR:CZ	2.38	0.59
1:B:32:ILE:O	1:B:36:VAL:HG23	2.03	0.58
1:D:32:ILE:O	1:D:36:VAL:HG23	2.03	0.58
1:D:466:GLU:OE2	1:D:526:LYS:NZ	2.35	0.58
1:B:383:ARG:HG3	1:B:430:TYR:HE2	1.69	0.58
1:D:14:PHE:O	1:D:18:ILE:HG13	2.04	0.57
1:A:256:LYS:NZ	1:A:259:TRP:CE3	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ALA:HB2	1:A:545:ILE:HD13	1.86	0.57
1:A:547:ARG:HG3	1:A:547:ARG:NH1	2.17	0.57
1:D:241:ARG:O	1:D:270:ALA:HB2	2.05	0.57
1:D:147:ASP:OD2	1:D:219:ARG:NH1	2.38	0.57
1:A:147:ASP:OD2	1:A:219:ARG:NH1	2.37	0.56
1:D:414:LEU:HB3	1:A:541:ILE:HG23	1.85	0.56
1:B:86:MET:HE2	1:B:114:MET:CE	2.35	0.56
1:A:134:THR:HB	1:A:159:ARG:NE	2.20	0.56
1:B:256:LYS:NZ	1:B:299:CYS:SG	2.71	0.56
1:B:485:VAL:CG2	1:B:493:LEU:HB2	2.36	0.56
1:B:435:ASP:HB3	1:B:447:PHE:HE1	1.71	0.56
1:C:93:THR:HA	1:C:190:GLU:HG3	1.89	0.55
1:C:325:VAL:CG1	1:C:350:PHE:CE1	2.88	0.55
1:C:147:ASP:OD2	1:C:219:ARG:NH1	2.39	0.55
1:C:112:HIS:CG	1:C:113:PRO:HD2	2.42	0.55
1:B:547:ARG:HH11	1:B:547:ARG:CG	2.14	0.55
1:A:153:ILE:C	1:A:153:ILE:HD12	2.32	0.55
1:C:309:ILE:HD13	1:C:335:VAL:HG22	1.88	0.55
1:D:66:ILE:HG12	1:D:77:LYS:HE3	1.88	0.54
1:D:134:THR:HB	1:D:159:ARG:CD	2.37	0.54
1:B:241:ARG:O	1:B:270:ALA:HB2	2.06	0.54
1:D:216:MET:HE3	1:D:217:PRO:HD2	1.90	0.54
1:D:490:ARG:HE	1:D:493:LEU:HD21	1.73	0.54
1:C:106:TYR:CD1	1:C:150:PRO:HB3	2.43	0.54
1:A:485:VAL:CG2	1:A:493:LEU:HB2	2.38	0.54
1:A:483:VAL:HB	1:A:551:ARG:NH1	2.23	0.54
1:C:287:LEU:HG	1:C:308:PHE:CD1	2.42	0.54
1:C:447:PHE:CE2	1:C:449:GLY:HA2	2.43	0.54
1:C:153:ILE:C	1:C:153:ILE:HD12	2.33	0.53
1:C:134:THR:HB	1:C:159:ARG:CD	2.38	0.53
1:B:13:PHE:CZ	1:B:36:VAL:HG22	2.43	0.53
1:C:283:THR:HG21	1:C:307:GLN:CB	2.34	0.53
1:D:13:PHE:CZ	1:D:36:VAL:HG22	2.42	0.53
1:D:210:THR:CG2	1:D:354:THR:HG21	2.39	0.53
1:B:40:ASP:OD1	1:B:42:ARG:HD3	2.09	0.53
1:D:544:LYS:NZ	1:A:388:GLU:HG2	2.24	0.53
1:B:106:TYR:CD1	1:B:150:PRO:HB3	2.44	0.53
1:D:114:MET:O	1:D:118:VAL:HG23	2.09	0.53
1:C:485:VAL:CG2	1:C:493:LEU:HB2	2.39	0.53
1:D:33:VAL:HG21	1:D:378:PRO:HB2	1.91	0.52
1:D:144:ARG:HG2	1:D:209:PHE:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:O	1:B:200:ARG:HG2	2.10	0.52
1:B:112:HIS:CG	1:B:113:PRO:HD2	2.44	0.52
1:B:249:LEU:HD13	1:B:286:TYR:CZ	2.44	0.52
1:D:470:ALA:O	1:D:518:MET:HE1	2.10	0.52
1:B:134:THR:HB	1:B:159:ARG:CD	2.40	0.52
1:B:144:ARG:HG2	1:B:209:PHE:CE2	2.45	0.52
1:D:249:LEU:HD13	1:D:286:TYR:CZ	2.45	0.52
1:B:70:ILE:O	1:B:70:ILE:HG22	2.10	0.52
1:A:326:SER:OG	1:A:331:LEU:HD22	2.09	0.51
1:B:485:VAL:HG22	1:B:493:LEU:HB2	1.92	0.51
1:D:153:ILE:C	1:D:153:ILE:HD12	2.36	0.51
1:D:53:ASP:OD1	1:D:57:LYS:HE3	2.10	0.51
1:B:457:THR:HG22	1:B:492:GLN:O	2.10	0.51
1:B:153:ILE:HD11	1:B:184:TRP:CH2	2.46	0.51
1:D:283:THR:HG21	1:D:307:GLN:HB3	1.93	0.51
1:A:259:TRP:HH2	1:A:352:GLY:HA3	1.76	0.51
1:C:144:ARG:HG2	1:C:209:PHE:CE2	2.46	0.51
1:D:159:ARG:HH11	1:D:159:ARG:HG3	1.76	0.50
1:D:447:PHE:CE2	1:D:449:GLY:HA2	2.46	0.50
1:A:248:ASN:HD21	1:A:250:SER:HB3	1.75	0.50
1:A:547:ARG:HH11	1:A:547:ARG:CG	2.10	0.50
1:C:241:ARG:O	1:C:270:ALA:HB2	2.12	0.50
1:B:131:PRO:HG2	1:B:208:TYR:CE1	2.45	0.50
1:A:379:LEU:HD23	1:A:379:LEU:O	2.12	0.50
1:B:466:GLU:OE2	1:B:526:LYS:NZ	2.35	0.50
1:A:346:THR:HG21	1:A:368:VAL:HG21	1.94	0.49
1:D:106:TYR:CD1	1:D:150:PRO:HB3	2.47	0.49
1:D:283:THR:HB	1:D:311:LEU:HD11	1.94	0.49
1:D:544:LYS:CE	1:A:388:GLU:HG2	2.42	0.49
1:A:115:HIS:CE1	1:A:252:THR:HB	2.47	0.49
1:A:200:ARG:HD2	1:A:202:GLU:OE2	2.13	0.49
1:D:53:ASP:OD1	1:D:57:LYS:CE	2.60	0.49
1:C:360:VAL:HG13	1:C:375:LYS:C	2.37	0.49
1:A:242:GLU:HG3	1:A:243:SER:N	2.27	0.49
1:B:147:ASP:OD2	1:B:219:ARG:NH1	2.41	0.49
1:A:485:VAL:HG22	1:A:493:LEU:HB2	1.95	0.49
1:D:299:CYS:HA	1:D:325:VAL:HG23	1.95	0.49
1:A:447:PHE:CE2	1:A:449:GLY:HA2	2.48	0.49
1:B:33:VAL:HG21	1:B:378:PRO:HB2	1.95	0.49
1:D:505:MET:HB3	1:D:506:PRO:HD2	1.94	0.48
1:C:284:ARG:HE	1:C:315:GLN:HE22	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:HB3	1:B:319:GLU:HG3	1.94	0.48
1:A:281:LEU:CD2	1:A:283:THR:HG22	2.42	0.48
1:D:296:THR:HG22	1:D:320:ARG:O	2.14	0.48
1:A:106:TYR:CD1	1:A:150:PRO:HB3	2.49	0.48
1:C:13:PHE:CZ	1:C:36:VAL:HG22	2.49	0.48
1:D:70:ILE:CG2	1:D:70:ILE:O	2.62	0.48
1:A:13:PHE:CZ	1:A:36:VAL:HG22	2.48	0.48
1:B:259:TRP:HH2	1:B:352:GLY:HA3	1.79	0.48
1:C:282:ASP:OD2	1:C:285:ARG:HD2	2.13	0.48
1:D:284:ARG:HH12	1:D:288:GLY:HA3	1.79	0.47
1:A:317:ARG:HD2	1:A:319:GLU:OE2	2.14	0.47
1:A:325:VAL:HG12	1:A:350:PHE:HE1	1.76	0.47
1:A:470:ALA:O	1:A:518:MET:HE1	2.14	0.47
1:C:216:MET:HB3	1:C:217:PRO:HD2	1.95	0.47
1:B:86:MET:HE2	1:B:114:MET:HE1	1.97	0.47
1:C:477:VAL:HG13	1:C:498:ILE:HG23	1.96	0.47
1:D:259:TRP:HH2	1:D:352:GLY:HA3	1.80	0.47
1:D:309:ILE:CD1	1:D:335:VAL:HG22	2.45	0.47
1:D:414:LEU:CB	1:A:541:ILE:CG2	2.90	0.47
1:A:11:GLN:HB3	1:A:15:ARG:NH2	2.29	0.47
1:B:256:LYS:HE2	1:B:350:PHE:CZ	2.49	0.47
1:C:247:LEU:CD2	1:C:290:VAL:HG22	2.45	0.47
1:D:119:PHE:HB3	1:D:262:PHE:CZ	2.49	0.47
1:A:86:MET:HE2	1:A:114:MET:HE2	1.97	0.47
1:C:325:VAL:HG12	1:C:350:PHE:HE1	1.80	0.47
1:C:457:THR:HG23	1:C:457:THR:O	2.15	0.47
1:A:281:LEU:CD2	1:A:283:THR:CG2	2.93	0.47
1:B:153:ILE:HD12	1:B:153:ILE:C	2.40	0.47
1:A:360:VAL:HG13	1:A:375:LYS:C	2.40	0.46
1:B:546:ARG:CZ	1:B:549:GLU:OE1	2.63	0.46
1:C:122:VAL:HG11	1:C:129:MET:HB2	1.97	0.46
1:C:256:LYS:HE3	1:C:256:LYS:HB2	1.66	0.46
1:C:470:ALA:O	1:C:518:MET:HE1	2.15	0.46
1:D:360:VAL:HG13	1:D:375:LYS:C	2.40	0.46
1:B:456:LYS:HB3	1:B:491:TRP:HD1	1.79	0.46
1:C:144:ARG:HG2	1:C:209:PHE:CD2	2.49	0.46
1:A:144:ARG:HG2	1:A:209:PHE:CE2	2.51	0.46
1:A:134:THR:HB	1:A:159:ARG:CD	2.45	0.46
1:C:317:ARG:HA	1:C:317:ARG:HD3	1.78	0.46
1:D:479:GLU:HB2	1:D:499:VAL:HB	1.97	0.46
1:D:26:GLU:O	1:D:29:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PHE:HB3	1:B:262:PHE:CZ	2.50	0.46
1:B:326:SER:HB3	1:B:331:LEU:HD22	1.98	0.46
1:B:248:ASN:HB3	1:B:261:SER:OG	2.15	0.46
1:C:26:GLU:O	1:C:29:LEU:HB3	2.15	0.46
1:A:26:GLU:O	1:A:29:LEU:HB3	2.16	0.45
1:D:493:LEU:HD23	1:D:493:LEU:HA	1.70	0.45
1:A:55:HIS:ND1	1:A:59:ARG:NH1	2.63	0.45
1:B:144:ARG:HG2	1:B:209:PHE:CD2	2.52	0.45
1:C:55:HIS:ND1	1:C:59:ARG:NH1	2.63	0.45
1:A:33:VAL:HG21	1:A:378:PRO:HB2	1.99	0.45
1:B:114:MET:O	1:B:118:VAL:HG23	2.16	0.45
1:D:144:ARG:HG2	1:D:209:PHE:CD2	2.51	0.45
1:D:159:ARG:HG3	1:D:159:ARG:NH1	2.31	0.45
1:A:234:THR:O	1:A:238:VAL:HG23	2.17	0.45
1:B:26:GLU:O	1:B:29:LEU:HB3	2.16	0.45
1:A:247:LEU:CD2	1:A:290:VAL:HG22	2.46	0.45
1:C:452:ASP:HB3	1:C:454:VAL:H	1.82	0.45
1:B:13:PHE:HE2	1:B:232:ILE:HD11	1.82	0.45
1:C:131:PRO:HG2	1:C:208:TYR:CE1	2.52	0.45
1:C:549:GLU:O	1:C:553:ARG:HG3	2.16	0.45
1:B:69:ASP:HB3	1:B:72:THR:OG1	2.16	0.45
1:A:159:ARG:HG3	1:A:159:ARG:HH11	1.81	0.44
1:B:470:ALA:O	1:B:518:MET:HE1	2.17	0.44
1:D:158:LEU:HD12	1:D:158:LEU:HA	1.79	0.44
1:C:309:ILE:CD1	1:C:335:VAL:HG22	2.48	0.44
1:D:112:HIS:CG	1:D:113:PRO:HD2	2.53	0.44
1:A:69:ASP:HB3	1:A:72:THR:OG1	2.17	0.44
1:A:112:HIS:CG	1:A:113:PRO:HD2	2.52	0.44
1:D:346:THR:HG21	1:D:368:VAL:HG21	2.00	0.44
1:C:401:ILE:HD11	1:C:437:ALA:HB2	1.99	0.44
1:B:216:MET:HE3	1:B:217:PRO:HD2	1.99	0.43
1:B:360:VAL:HG13	1:B:375:LYS:C	2.43	0.43
1:C:435:ASP:OD1	2:C:601:AMP:O2'	2.32	0.43
1:C:216:MET:HE3	1:C:217:PRO:HD2	2.00	0.43
1:D:309:ILE:HD13	1:D:335:VAL:HG22	1.99	0.43
1:C:114:MET:O	1:C:118:VAL:HG23	2.18	0.43
1:C:231:SER:HB2	1:C:267:LEU:HD11	1.98	0.43
1:D:401:ILE:HD11	1:D:437:ALA:HB2	2.00	0.43
1:A:89:ARG:HG3	1:A:192:SER:CB	2.48	0.43
1:A:287:LEU:HG	1:A:308:PHE:CE1	2.54	0.43
1:A:317:ARG:CD	1:A:319:GLU:OE2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ILE:HD13	1:B:335:VAL:HG22	1.98	0.43
1:C:247:LEU:HD23	1:C:290:VAL:HG22	1.99	0.43
1:C:287:LEU:HG	1:C:308:PHE:CE1	2.53	0.43
1:D:46:TRP:HE1	1:D:267:LEU:CD2	2.30	0.43
1:A:144:ARG:HG2	1:A:209:PHE:CD2	2.53	0.43
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.82	0.43
1:C:119:PHE:HB3	1:C:262:PHE:CZ	2.54	0.43
1:B:256:LYS:HE2	1:B:350:PHE:HZ	1.83	0.43
1:C:69:ASP:HB3	1:C:72:THR:OG1	2.19	0.43
1:C:226:SER:O	1:C:411:GLY:HA2	2.19	0.43
1:D:211:SER:HB3	1:D:463:GLY:N	2.34	0.42
1:B:558:ARG:O	1:C:178:ASP:HA	2.19	0.42
1:A:119:PHE:HB3	1:A:262:PHE:CZ	2.54	0.42
1:B:408:ARG:NH2	1:B:413:PHE:O	2.51	0.42
1:B:159:ARG:HG3	1:B:159:ARG:HH11	1.84	0.42
1:D:210:THR:HG21	1:D:354:THR:CG2	2.49	0.42
1:A:309:ILE:CD1	1:A:335:VAL:HG22	2.49	0.42
1:A:324:VAL:C	1:A:325:VAL:HG23	2.43	0.42
1:B:70:ILE:O	1:B:70:ILE:CG2	2.66	0.42
1:D:414:LEU:HD23	1:D:414:LEU:HA	1.87	0.42
1:B:296:THR:HG22	1:B:320:ARG:O	2.19	0.42
1:D:547:ARG:HH11	1:D:547:ARG:CG	2.18	0.42
1:A:174:LYS:NZ	1:A:183:THR:OG1	2.52	0.42
1:A:530:ILE:HG12	1:A:569:VAL:HG13	2.01	0.42
1:B:44:PHE:O	1:B:199:THR:OG1	2.34	0.42
1:B:546:ARG:NH2	1:B:549:GLU:OE1	2.53	0.42
1:D:414:LEU:CB	1:A:541:ILE:HG21	2.45	0.42
1:B:246:HIS:HA	1:B:297:SER:O	2.20	0.42
1:D:44:PHE:O	1:D:199:THR:OG1	2.32	0.42
1:D:296:THR:HA	1:D:321:LEU:HA	2.01	0.42
1:D:264:SER:N	1:D:265:PRO:HD2	2.35	0.42
1:A:377:HIS:HA	1:A:378:PRO:HD3	1.92	0.42
1:A:159:ARG:HG3	1:A:159:ARG:NH1	2.33	0.42
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.84	0.42
1:D:153:ILE:HD11	1:D:184:TRP:CH2	2.55	0.41
1:A:406:ASN:HA	1:A:407:PRO:HA	1.95	0.41
1:B:264:SER:N	1:B:265:PRO:HD2	2.35	0.41
1:B:302:PRO:HD2	1:B:329:GLU:HG3	2.01	0.41
1:D:14:PHE:CE1	1:D:232:ILE:HD11	2.46	0.41
1:D:115:HIS:CE1	1:D:252:THR:HB	2.55	0.41
1:C:377:HIS:HA	1:C:378:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:MET:HE3	1:A:217:PRO:HD2	2.02	0.41
1:A:498:ILE:O	1:A:533:PHE:HA	2.20	0.41
1:D:131:PRO:HG2	1:D:208:TYR:CE1	2.54	0.41
1:D:256:LYS:NZ	1:D:299:CYS:SG	2.63	0.41
1:B:284:ARG:HG2	1:B:315:GLN:HE22	1.85	0.41
1:C:324:VAL:C	1:C:325:VAL:HG23	2.44	0.41
1:D:109:THR:O	1:D:252:THR:HG21	2.20	0.41
1:D:69:ASP:HB3	1:D:72:THR:OG1	2.20	0.41
1:D:108:MET:CE	1:D:159:ARG:HB3	2.49	0.41
1:D:475:PRO:O	1:D:501:LYS:HD2	2.20	0.41
1:B:159:ARG:HG3	1:B:159:ARG:NH1	2.36	0.41
1:A:226:SER:O	1:A:411:GLY:HA2	2.21	0.41
1:B:256:LYS:HE3	1:B:327:ALA:HB3	2.02	0.41
1:B:379:LEU:HD23	1:B:379:LEU:O	2.20	0.41
1:B:450:ARG:HD2	1:B:454:VAL:HB	2.02	0.41
1:D:42:ARG:O	1:D:200:ARG:HG2	2.21	0.41
1:A:63:THR:HG22	1:A:271:THR:HG23	2.03	0.41
1:C:153:ILE:HD11	1:C:184:TRP:CH2	2.55	0.41
1:D:216:MET:HB3	1:D:217:PRO:HD2	2.02	0.41
1:D:476:ALA:HA	1:D:504:TYR:CE2	2.56	0.41
1:D:484:GLY:HA2	1:D:493:LEU:O	2.21	0.41
1:A:309:ILE:HD13	1:A:335:VAL:HG22	2.03	0.41
1:B:424:GLU:O	1:B:427:ARG:NH1	2.46	0.41
1:C:36:VAL:HA	1:C:39:LEU:HD12	2.03	0.41
1:C:408:ARG:NH2	1:C:413:PHE:O	2.53	0.41
1:D:377:HIS:HA	1:D:378:PRO:HD3	1.95	0.41
1:A:114:MET:O	1:A:118:VAL:HG23	2.21	0.41
1:A:349:ASP:OD1	1:A:373:MET:HA	2.21	0.41
1:B:17:PHE:O	1:B:20:PHE:HB3	2.21	0.41
1:B:414:LEU:HD23	1:B:414:LEU:HA	1.87	0.41
1:B:475:PRO:O	1:B:501:LYS:HD2	2.21	0.41
1:B:486:PRO:O	1:B:558:ARG:NH2	2.51	0.40
1:C:485:VAL:HG23	1:C:493:LEU:HB2	2.02	0.40
1:B:377:HIS:HA	1:B:378:PRO:HD3	1.92	0.40
1:C:89:ARG:HA	1:C:191:SER:O	2.22	0.40
1:A:420:LYS:HA	1:A:423:MET:HE3	2.02	0.40
1:C:414:LEU:HD23	1:C:414:LEU:HA	1.85	0.40
1:D:230:GLY:HA3	1:D:357:THR:HG21	2.04	0.40
1:D:150:PRO:HG2	1:D:172:VAL:HG11	2.02	0.40
1:A:11:GLN:HB3	1:A:15:ARG:CZ	2.51	0.40
1:A:64:ALA:HA	1:A:80:TYR:CE1	2.57	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	560/570 (98%)	534 (95%)	26 (5%)	0	100	100
1	B	559/570 (98%)	534 (96%)	25 (4%)	0	100	100
1	C	550/570 (96%)	525 (96%)	25 (4%)	0	100	100
1	D	559/570 (98%)	532 (95%)	27 (5%)	0	100	100
All	All	2228/2280 (98%)	2125 (95%)	103 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	494/502 (98%)	478 (97%)	16 (3%)	34	70
1	B	493/502 (98%)	470 (95%)	23 (5%)	23	57
1	C	487/502 (97%)	471 (97%)	16 (3%)	33	69
1	D	493/502 (98%)	472 (96%)	21 (4%)	26	60
All	All	1967/2008 (98%)	1891 (96%)	76 (4%)	28	64

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	33	VAL
1	D	68	ARG
1	D	99	LEU
1	D	149	LYS
1	D	153	ILE
1	D	202	GLU
1	D	214	THR
1	D	252	THR
1	D	284	ARG
1	D	285	ARG
1	D	287	LEU
1	D	325	VAL
1	D	326	SER
1	D	329	GLU
1	D	332	ASN
1	D	413	PHE
1	D	420	LYS
1	D	507	SER
1	D	529	ARG
1	D	536	GLU
1	D	548	VAL
1	A	33	VAL
1	A	99	LEU
1	A	109	THR
1	A	153	ILE
1	A	232	ILE
1	A	242	GLU
1	A	329	GLU
1	A	332	ASN
1	A	349	ASP
1	A	404	LYS
1	A	413	PHE
1	A	441	GLU
1	A	448	VAL
1	A	493	LEU
1	A	517	LYS
1	A	542	SER
1	B	33	VAL
1	B	68	ARG
1	B	99	LEU
1	B	109	THR
1	B	153	ILE
1	B	232	ILE

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Mol	Chain	Res	Type
1	B	249	LEU
1	B	252	THR
1	B	260	SER
1	B	285	ARG
1	B	325	VAL
1	B	326	SER
1	B	329	GLU
1	B	346	THR
1	B	353	GLN
1	B	379	LEU
1	B	390	LYS
1	B	413	PHE
1	B	472	LEU
1	B	507	SER
1	B	536	GLU
1	B	542	SER
1	B	548	VAL
1	C	12	ASP
1	C	99	LEU
1	C	109	THR
1	C	192	SER
1	C	232	ILE
1	C	256	LYS
1	C	260	SER
1	C	287	LEU
1	C	326	SER
1	C	329	GLU
1	C	332	ASN
1	C	413	PHE
1	C	420	LYS
1	C	536	GLU
1	C	548	VAL
1	C	549	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	25	ASN
1	D	185	ASN
1	D	315	GLN
1	D	566	ASN
1	A	307	GLN

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Mol	Chain	Res	Type
1	A	315	GLN
1	A	400	HIS
1	B	25	ASN
1	B	315	GLN
1	B	566	ASN
1	C	25	ASN
1	C	307	GLN
1	C	315	GLN
1	C	400	HIS
1	C	566	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	AMP	A	601	-	25,25,25	0.61	0	37,38,38	0.98	1 (2%)
2	AMP	D	601	-	25,25,25	0.61	0	37,38,38	1.01	1 (2%)
2	AMP	C	601	-	25,25,25	0.60	1 (4%)	37,38,38	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6R9	B	601	-	27,28,28	0.60	1 (3%)	39,42,42	1.01	2 (5%)

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	AMP	A	601	-	-	4/10/26/26	0/3/3/3
2	AMP	D	601	-	-	0/10/26/26	0/3/3/3
2	AMP	C	601	-	-	0/10/26/26	0/3/3/3
3	6R9	B	601	-	-	0/13/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	AMP	P-O1P	2.10	1.57	1.50
3	B	601	6R9	P05-O04	2.06	1.64	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	6R9	O07-P05-O04	3.53	116.36	104.94
3	B	601	6R9	O04-P05-O08	-2.53	95.39	103.00
2	D	601	AMP	O3'-C3'-C4'	-2.27	104.56	111.08
2	A	601	AMP	O2'-C2'-C1'	2.25	117.87	110.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

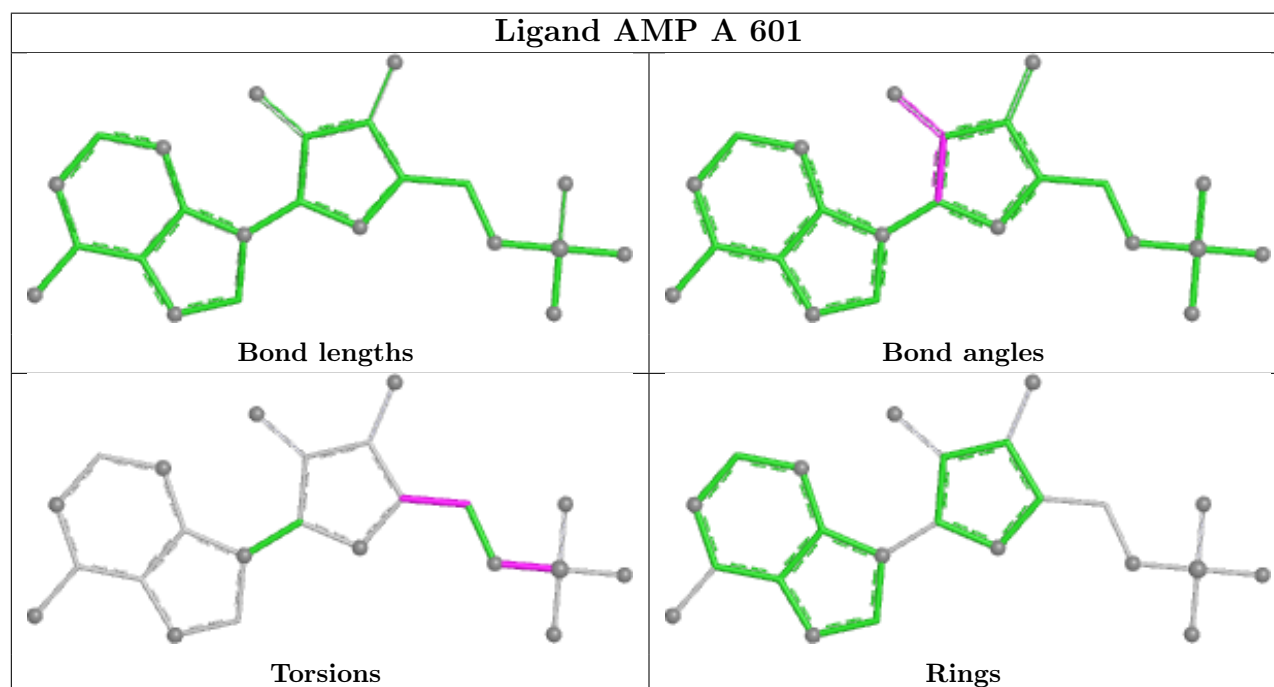
Mol	Chain	Res	Type	Atoms
2	A	601	AMP	C5'-O5'-P-O2P
2	A	601	AMP	C5'-O5'-P-O3P
2	A	601	AMP	C3'-C4'-C5'-O5'
2	A	601	AMP	O4'-C4'-C5'-O5'

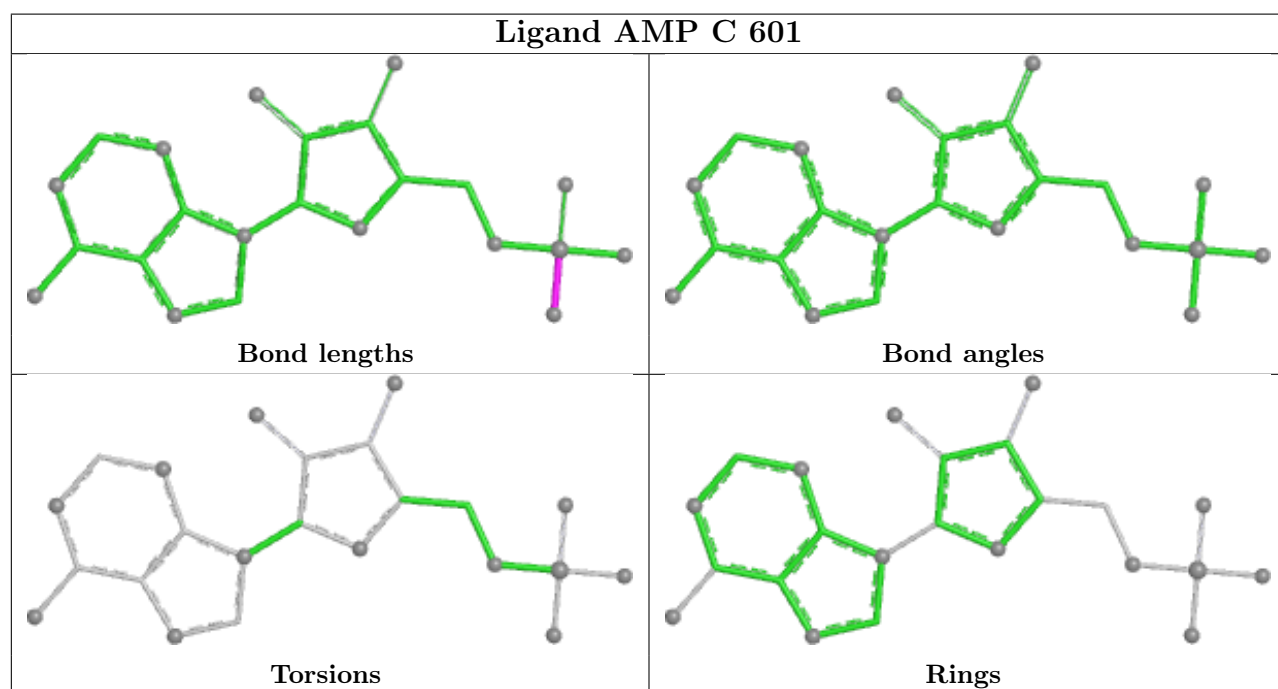
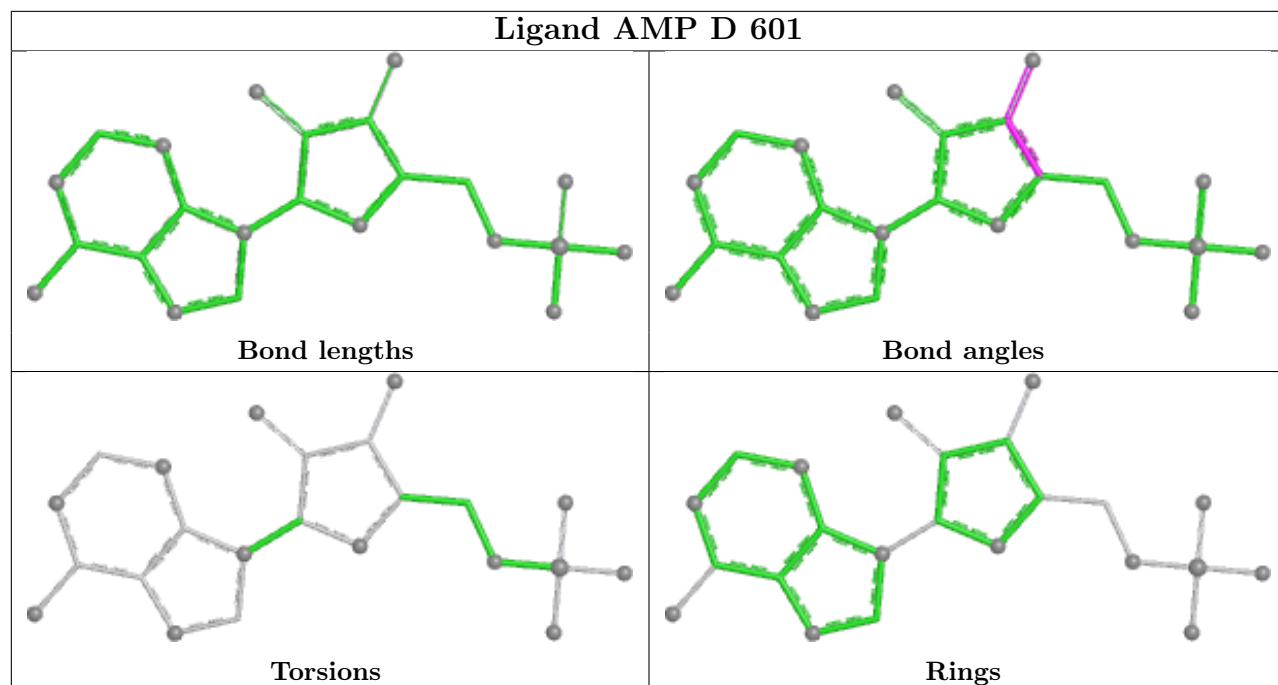
There are no ring outliers.

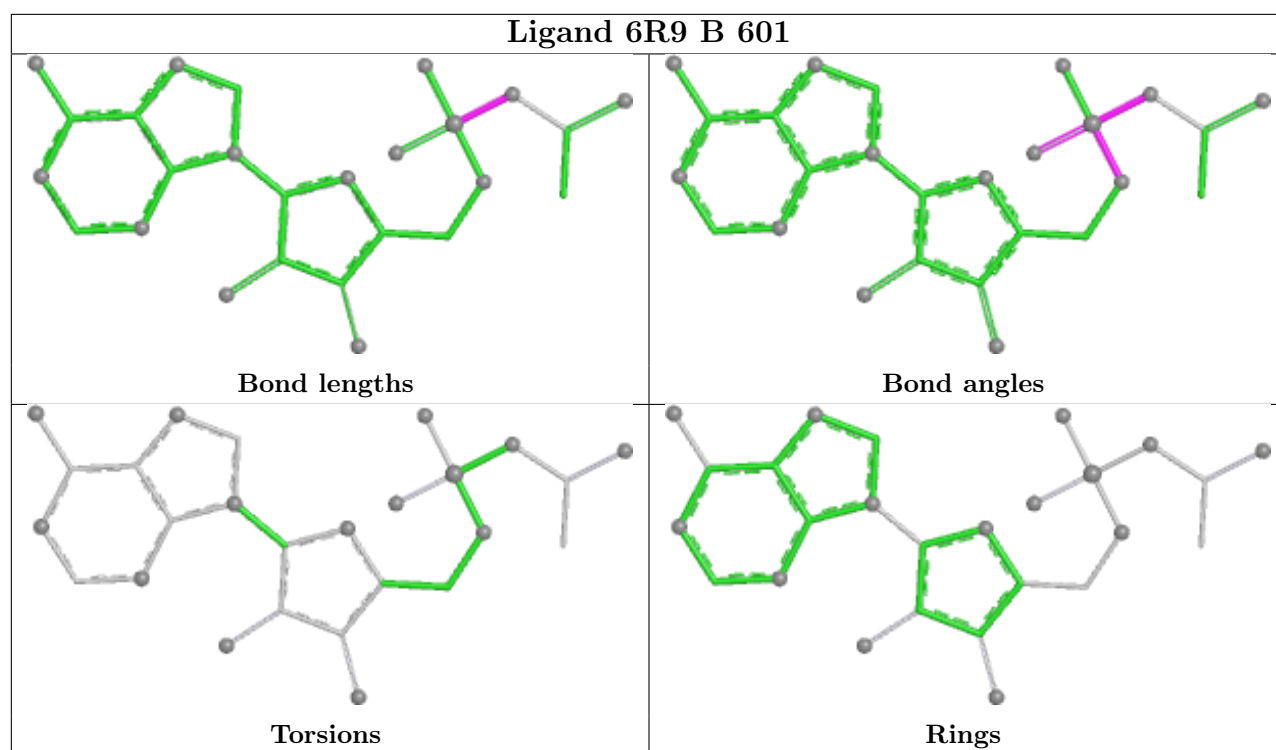
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	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 [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	562/570 (98%)	0.02	13 (2%) 61 51	37, 50, 75, 112	0
1	B	561/570 (98%)	0.13	14 (2%) 58 48	41, 57, 84, 100	0
1	C	554/570 (97%)	0.32	14 (2%) 58 48	46, 64, 97, 140	0
1	D	561/570 (98%)	0.19	10 (1%) 67 58	44, 61, 85, 104	0
All	All	2238/2280 (98%)	0.16	51 (2%) 61 51	37, 58, 86, 140	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	VAL	4.7
1	A	352	GLY	4.7
1	C	36	VAL	4.5
1	B	290	VAL	4.3
1	C	10	VAL	4.2
1	C	387	ASP	3.7
1	B	565	GLN	3.7
1	C	352	GLY	3.6
1	A	256	LYS	3.6
1	B	10	VAL	3.4
1	C	31	GLU	3.4
1	C	388	GLU	3.3
1	A	14	PHE	3.3
1	C	305	TRP	3.3
1	C	14	PHE	3.2
1	D	214	THR	3.2
1	B	563	VAL	2.9
1	A	31	GLU	2.8
1	B	560	LYS	2.7
1	D	541	ILE	2.6
1	A	178	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	231	SER	2.5
1	D	57	LYS	2.5
1	B	214	THR	2.5
1	C	179	GLY	2.4
1	C	17	PHE	2.4
1	D	149	LYS	2.4
1	A	210	THR	2.4
1	A	10	VAL	2.3
1	B	566	ASN	2.3
1	B	132	SER	2.3
1	A	73	GLY	2.3
1	B	274	GLY	2.3
1	B	148	LEU	2.3
1	D	277	TYR	2.3
1	C	252	THR	2.2
1	D	106	TYR	2.2
1	A	214	THR	2.2
1	D	150	PRO	2.2
1	A	389	GLY	2.2
1	C	243	SER	2.1
1	C	11	GLN	2.1
1	D	558	ARG	2.1
1	A	424	GLU	2.1
1	B	287	LEU	2.1
1	A	194	ALA	2.1
1	B	266	LEU	2.1
1	B	312	ASP	2.1
1	D	19	GLU	2.0
1	B	466	GLU	2.0
1	A	229	VAL	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 ⓘ

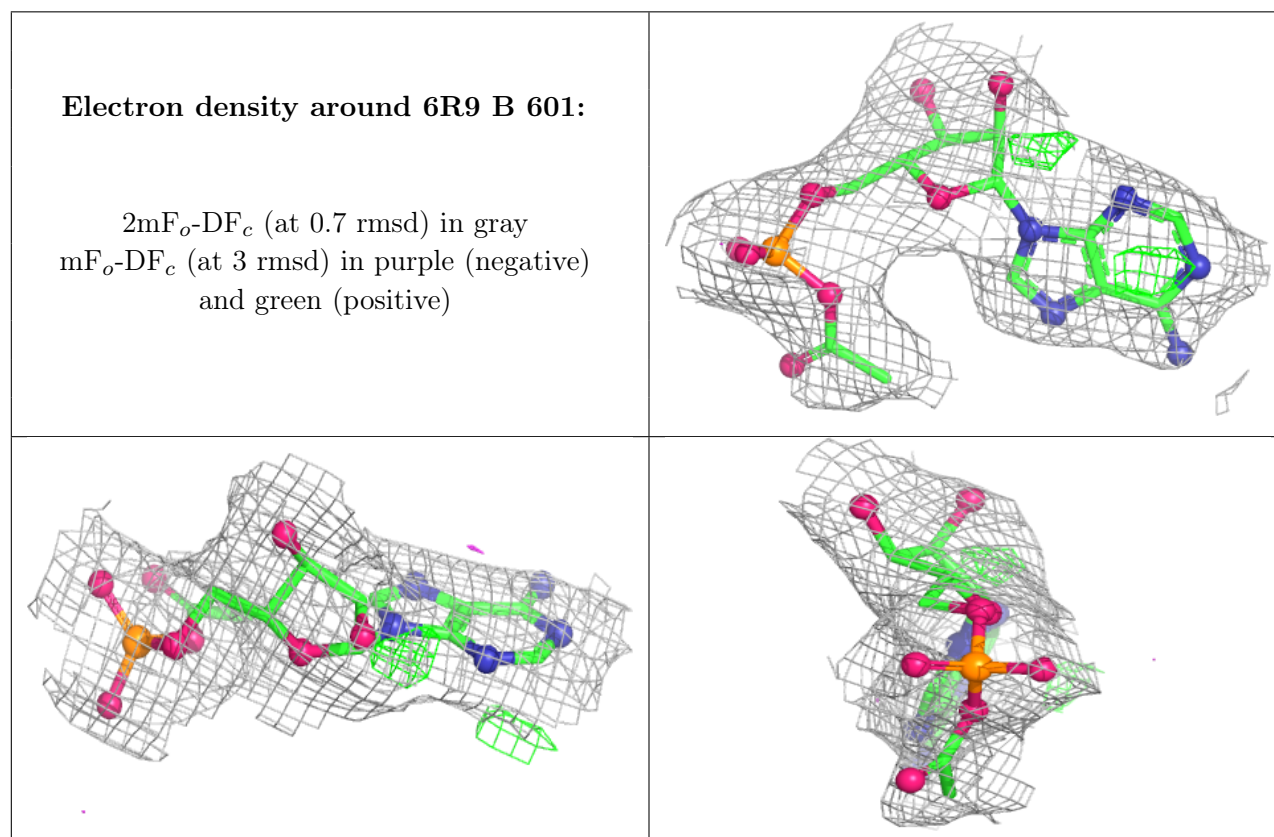
There are no oligosaccharides in this entry.

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.

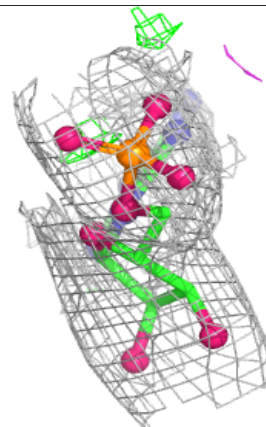
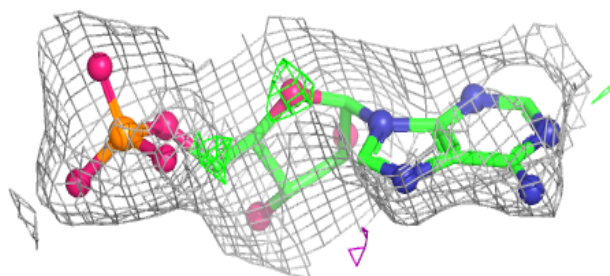
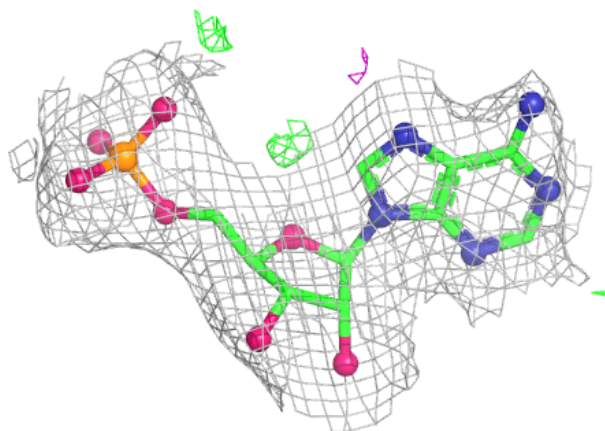
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	6R9	B	601	26/26	0.94	0.10	42,45,56,62	0
2	AMP	A	601	23/23	0.96	0.07	41,43,55,57	0
2	AMP	C	601	23/23	0.96	0.07	49,52,57,59	0
2	AMP	D	601	23/23	0.96	0.06	42,45,50,52	0

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.



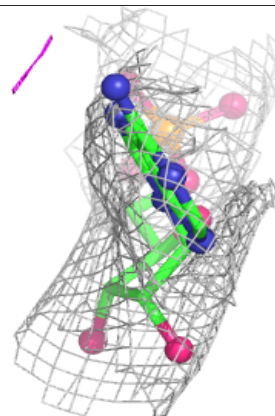
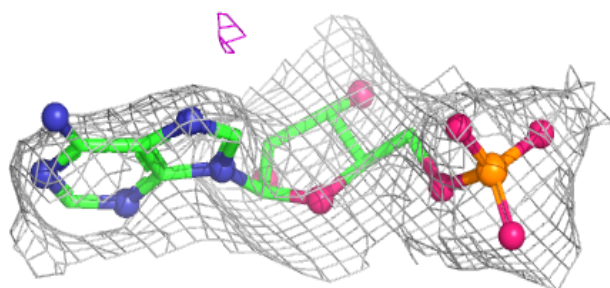
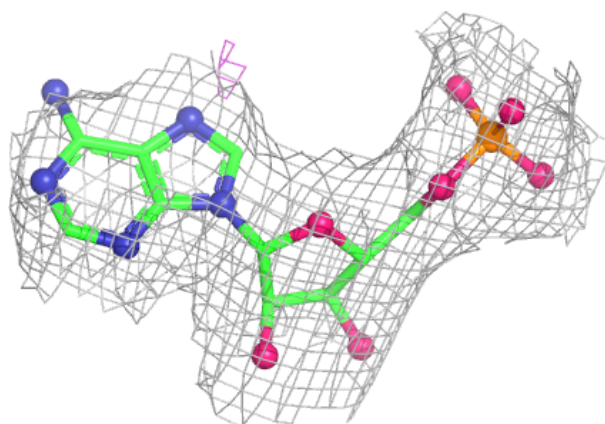
Electron density around AMP A 601:

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

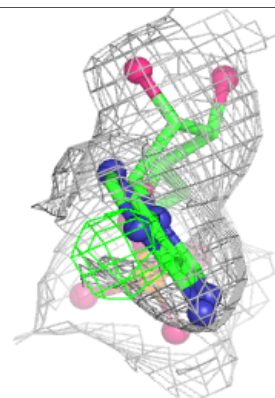
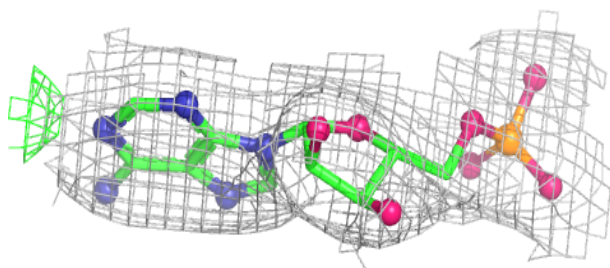
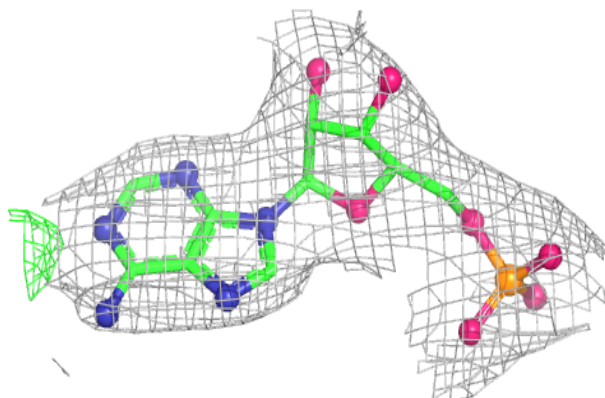


Electron density around AMP C 601:

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

**Electron density around AMP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.