Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 03:28 pm GMT

PDB ID	:	8BIQ
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:

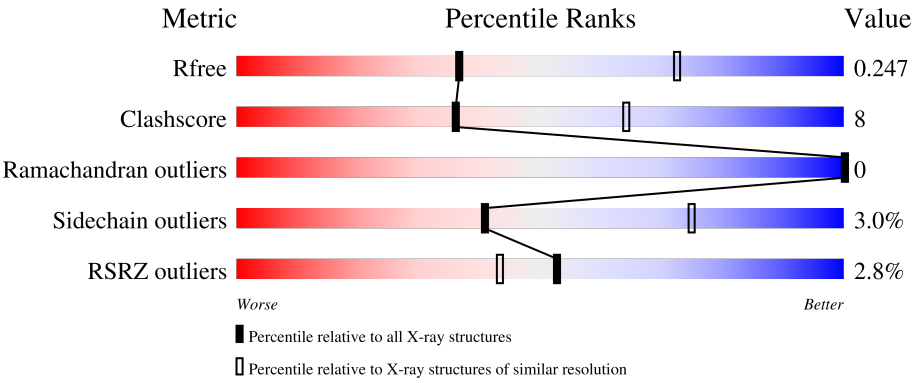
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	77% 20%
1	B	570	3% 78% 17%
1	C	570	4% 78% 18%
1	D	570	3% 76% 20%

2 Entry composition (i)

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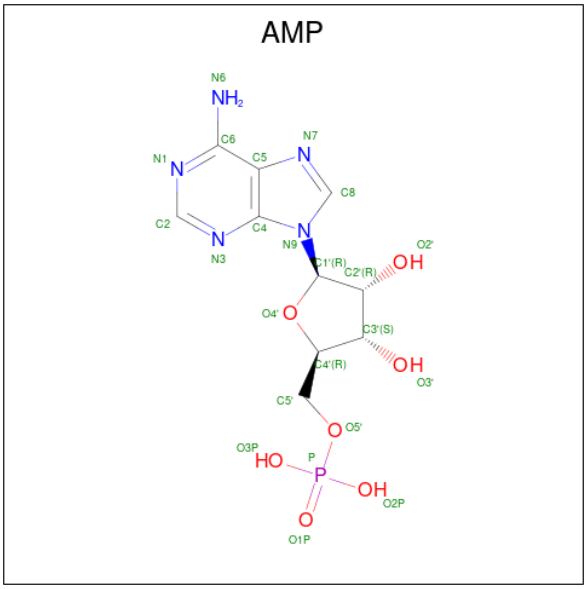
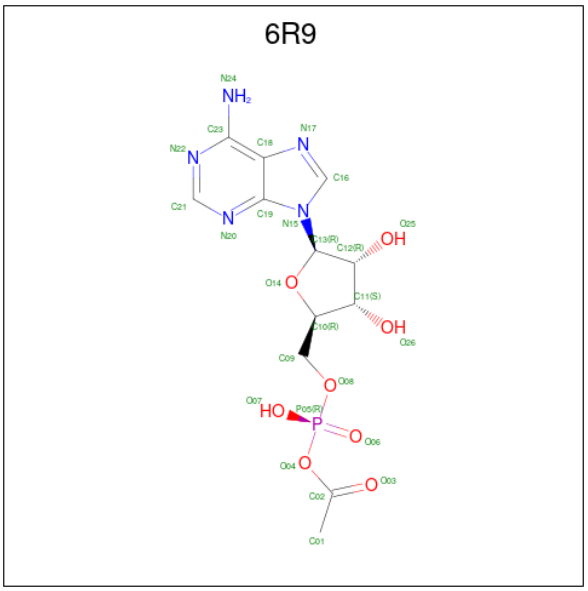
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A4YDT1
C	2	HIS	-	expression tag	UNP A4YDT1
C	3	HIS	-	expression tag	UNP A4YDT1
C	4	HIS	-	expression tag	UNP A4YDT1
C	5	HIS	-	expression tag	UNP A4YDT1
C	6	HIS	-	expression tag	UNP A4YDT1
C	7	HIS	-	expression tag	UNP A4YDT1

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: 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 (three-letter code: 6R9) (formula: $C_{12}H_{16}N_5O_8P$) (labeled as "Ligand of Interest" by depositor).



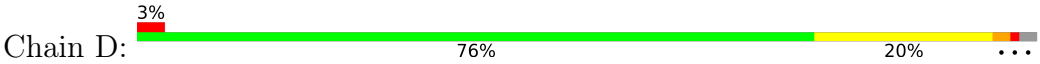
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			26	12	5	8	1		

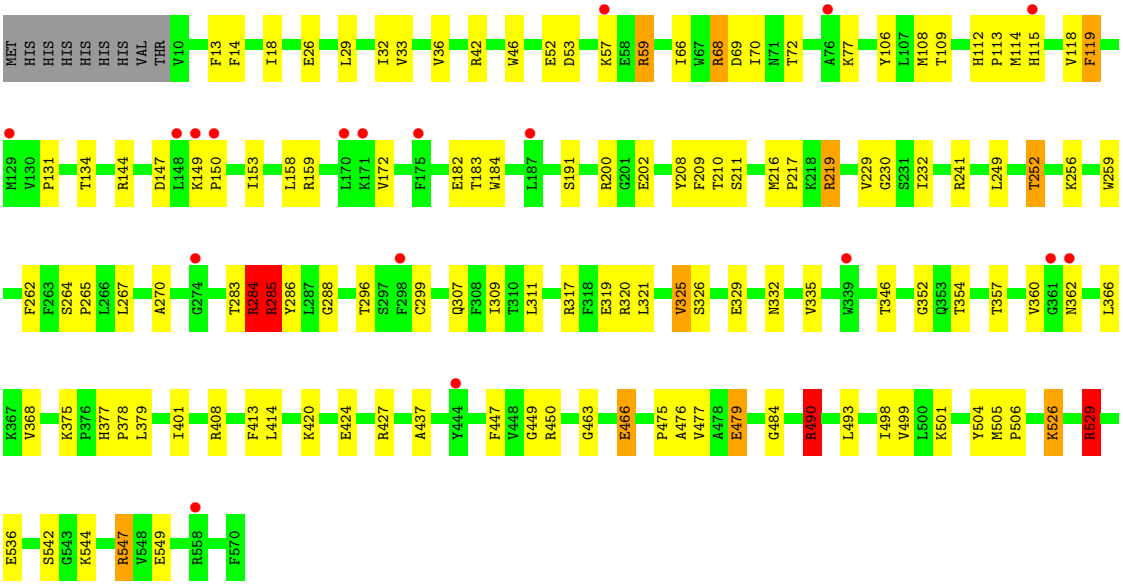
3 Residue-property plots (i)

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: 4-hydroxybutyrate--CoA ligase 1

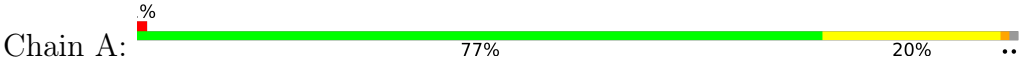
Chain D:

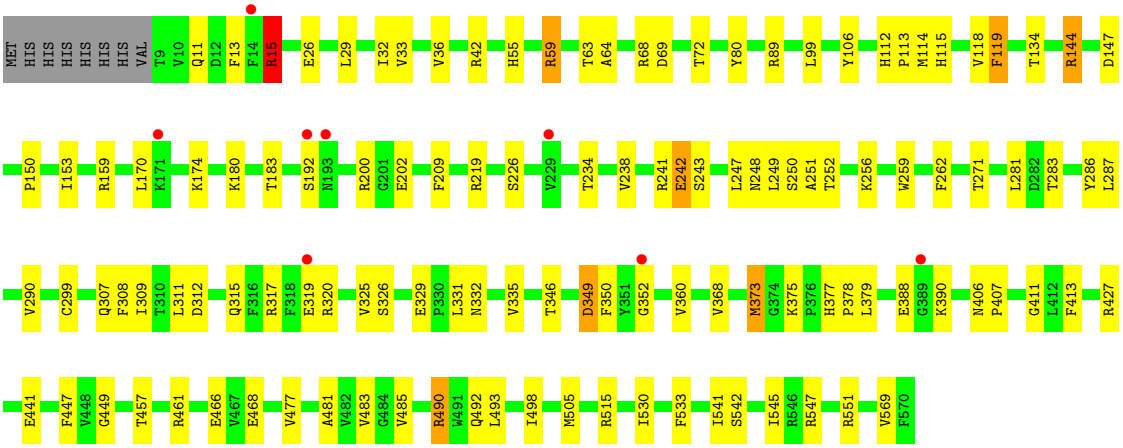




• Molecule 1: 4-hydroxybutyrate--CoA ligase 1

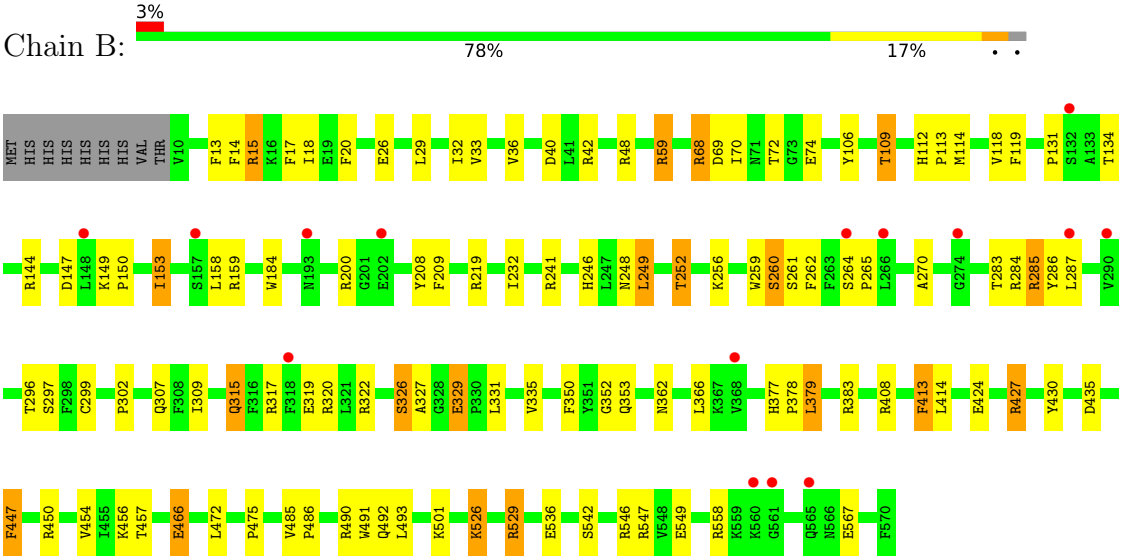
Chain A:





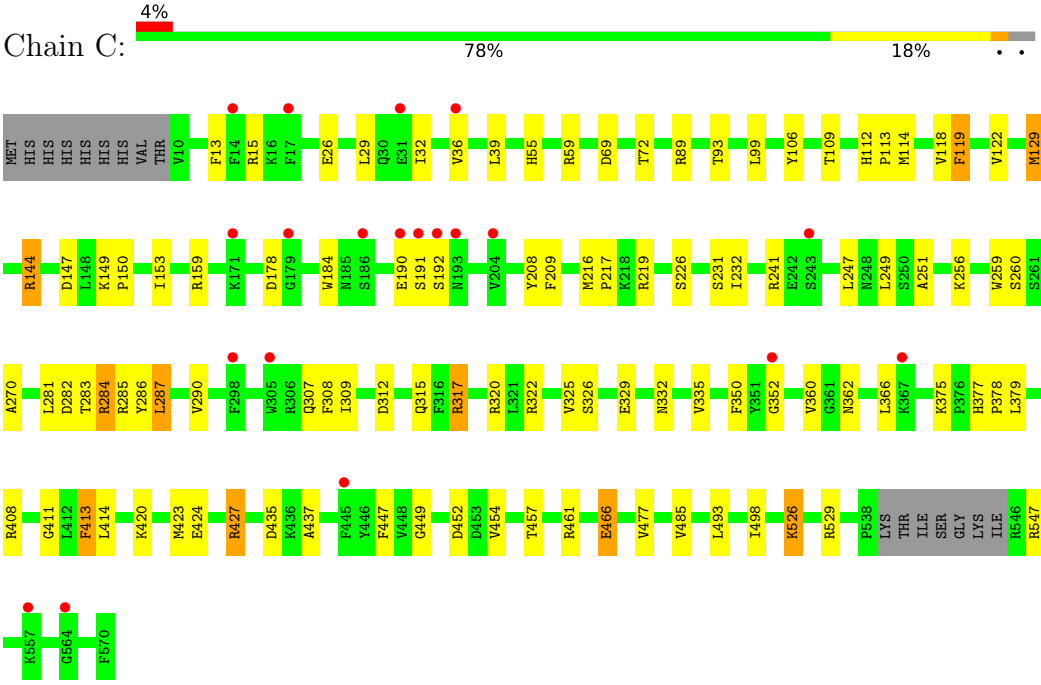
• Molecule 1: 4-hydroxybutyrate--CoA ligase 1

Chain B:



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

Chain C:



4 Data and refinement statistics (i)

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 66.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.48-2.80) 99.7 (66.39-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	2941 reflections (5.18%)	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)	0.27 , 0.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.60	0/4631	1.13	18/6257 (0.3%)
1	B	0.57	1/4624 (0.0%)	1.08	12/6247 (0.2%)
1	C	0.53	0/4572	1.07	14/6177 (0.2%)
1	D	0.56	1/4624 (0.0%)	1.05	11/6247 (0.2%)
All	All	0.56	2/18451 (0.0%)	1.08	55/24928 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	GLU	CD-OE1	6.12	1.32	1.25
1	D	479	GLU	CD-OE2	5.43	1.31	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	490	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	A	461	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	C	461	ARG	NE-CZ-NH1	8.41	124.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	529	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	A	490	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	D	408	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	A	68	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	180	LYS	CB-CA-C	-7.32	95.77	110.40
1	C	427	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	322	ARG	CG-CD-NE	-6.72	97.70	111.80
1	D	529	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	505	MET	CG-SD-CE	6.69	110.90	100.20
1	A	15	ARG	CB-CA-C	6.50	123.40	110.40
1	D	59	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	149	LYS	CB-CG-CD	6.43	128.31	111.60
1	B	59	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	526	LYS	CD-CE-NZ	-6.29	97.23	111.70
1	A	468	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	B	285	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	466	GLU	N-CA-CB	-6.09	99.64	110.60
1	D	549	GLU	OE1-CD-OE2	5.98	130.48	123.30
1	A	515	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	15	ARG	CB-CA-C	5.93	122.27	110.40
1	A	241	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	299	CYS	CB-CA-C	-5.88	98.65	110.40
1	C	461	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	315	GLN	CB-CA-C	-5.76	98.88	110.40
1	C	317	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	D	526	LYS	CD-CE-NZ	-5.74	98.50	111.70
1	C	466	GLU	N-CA-CB	-5.73	100.29	110.60
1	C	423	MET	CG-SD-CE	5.69	109.31	100.20
1	B	526	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	C	15	ARG	CB-CA-C	5.66	121.72	110.40
1	B	447	PHE	CB-CA-C	-5.59	99.23	110.40
1	A	311	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	D	466	GLU	N-CA-CB	-5.53	100.65	110.60
1	D	466	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	A	461	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	450	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	567	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	C	529	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	529	ARG	CG-CD-NE	-5.30	100.66	111.80
1	C	322	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	59	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	74	GLU	OE1-CD-OE2	5.27	129.63	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	149	LYS	CD-CE-NZ	5.17	123.58	111.70
1	A	42	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	129	MET	CG-SD-CE	5.13	108.40	100.20
1	D	219	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	466	GLU	CG-CD-OE2	-5.12	108.07	118.30
1	C	281	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	373	MET	CG-SD-CE	-5.09	92.06	100.20
1	B	149	LYS	CB-CG-CD	5.07	124.78	111.60
1	A	315	GLN	CB-CA-C	-5.04	100.32	110.40
1	A	170	LEU	CB-CG-CD1	5.03	119.55	111.00

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4526	0	4542	78	0
1	B	4519	0	4535	69	0
1	C	4468	0	4471	60	0
1	D	4519	0	4535	91	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	288	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 (288) 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: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:D:379:LEU:HD23	1:D:379:LEU:O	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:466:GLU:OE2	1:D:526:LYS:NZ	2.35	0.57
1:A:256:LYS:NZ	1:A:259:TRP:CE3	2.68	0.57
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:A:134:THR:HB	1:A:159:ARG:NE	2.20	0.56
1:B:485:VAL:CG2	1:B:493:LEU:HB2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:466:GLU:OE2	1:C:526:LYS:NZ	2.33	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:153:ILE:C	1:A:153:ILE:HD12	2.32	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: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:C:153:ILE:C	1:C:153:ILE:HD12	2.33	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
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:C:216:MET:HB3	1:C:217:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:256:LYS:NZ	1:B:299:CYS:SG	2.71	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: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:D:153:ILE:C	1:D:153:ILE:HD12	2.36	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
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:B:256:LYS:NZ	1:B:260:SER:OG	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:360:VAL:HG13	1:C:375:LYS:C	2.37	0.45
1:A:159:ARG:HG3	1:A:159:ARG:HH11	1.81	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: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
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:C:435:ASP:OD1	2:C:601:AMP:O2'	2.32	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:D:108:MET:CE	1:D:159:ARG:HB3	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:153:ILE:HD12	1:B:153:ILE:C	2.40	0.42
1:B:246:HIS:HA	1:B:297:SER:O	2.20	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:360:VAL:HG13	1:A:375:LYS:C	2.40	0.42
1:A:377:HIS:HA	1:A:378:PRO:HD3	1.92	0.42
1:D:360:VAL:HG13	1:D:375:LYS:C	2.40	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:182:GLU:O	1:D:183:THR:OG1	2.37	0.40
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: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%)	483 (98%)	11 (2%)	52	83
1	B	493/502 (98%)	477 (97%)	16 (3%)	39	73
1	C	487/502 (97%)	471 (97%)	16 (3%)	38	72
1	D	493/502 (98%)	477 (97%)	16 (3%)	39	73
All	All	1967/2008 (98%)	1908 (97%)	59 (3%)	41	75

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	68	ARG
1	D	119	PHE
1	D	149	LYS
1	D	191	SER
1	D	202	GLU
1	D	252	THR
1	D	284	ARG
1	D	285	ARG
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	529	ARG
1	D	536	GLU
1	A	99	LEU
1	A	119	PHE
1	A	144	ARG
1	A	242	GLU
1	A	312	ASP
1	A	329	GLU

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Mol	Chain	Res	Type
1	A	332	ASN
1	A	349	ASP
1	A	413	PHE
1	A	441	GLU
1	A	542	SER
1	B	68	ARG
1	B	109	THR
1	B	153	ILE
1	B	249	LEU
1	B	252	THR
1	B	260	SER
1	B	285	ARG
1	B	326	SER
1	B	329	GLU
1	B	353	GLN
1	B	379	LEU
1	B	413	PHE
1	B	472	LEU
1	B	529	ARG
1	B	536	GLU
1	B	542	SER
1	C	99	LEU
1	C	109	THR
1	C	119	PHE
1	C	144	ARG
1	C	192	SER
1	C	232	ILE
1	C	260	SER
1	C	287	LEU
1	C	312	ASP
1	C	326	SER
1	C	329	GLU
1	C	332	ASN
1	C	413	PHE
1	C	420	LYS
1	C	548	VAL
1	C	549	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	315	GLN

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Mol	Chain	Res	Type
1	A	315	GLN
1	B	315	GLN
1	C	315	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	-	22,25,25	0.79	0	25,38,38	1.17	2 (8%)
2	AMP	D	601	-	22,25,25	0.91	0	25,38,38	1.07	1 (4%)
3	6R9	B	601	-	24,28,28	0.83	0	26,42,42	1.39	3 (11%)
2	AMP	C	601	-	22,25,25	0.78	1 (4%)	25,38,38	1.03	2 (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	AMP	A	601	-	-	4/6/26/26	0/3/3/3
2	AMP	D	601	-	-	0/6/26/26	0/3/3/3
3	6R9	B	601	-	-	1/9/31/31	0/3/3/3
2	AMP	C	601	-	-	0/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	AMP	P-O1P	2.00	1.57	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	6R9	O07-P05-O04	3.74	116.36	104.14
3	B	601	6R9	C18-C23-N24	2.86	124.69	120.35
3	B	601	6R9	O04-P05-O08	-2.58	95.39	102.92
2	C	601	AMP	C3'-C2'-C1'	2.32	104.47	100.98
2	A	601	AMP	O4'-C1'-C2'	2.26	110.23	106.93
2	D	601	AMP	O3'-C3'-C4'	-2.24	104.56	111.05
2	C	601	AMP	C5-C6-N6	2.10	123.54	120.35
2	A	601	AMP	C5-C6-N6	2.01	123.40	120.35

There are no chirality outliers.

All (5) 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'
3	B	601	6R9	C02-O04-P05-O06

There are no ring outliers.

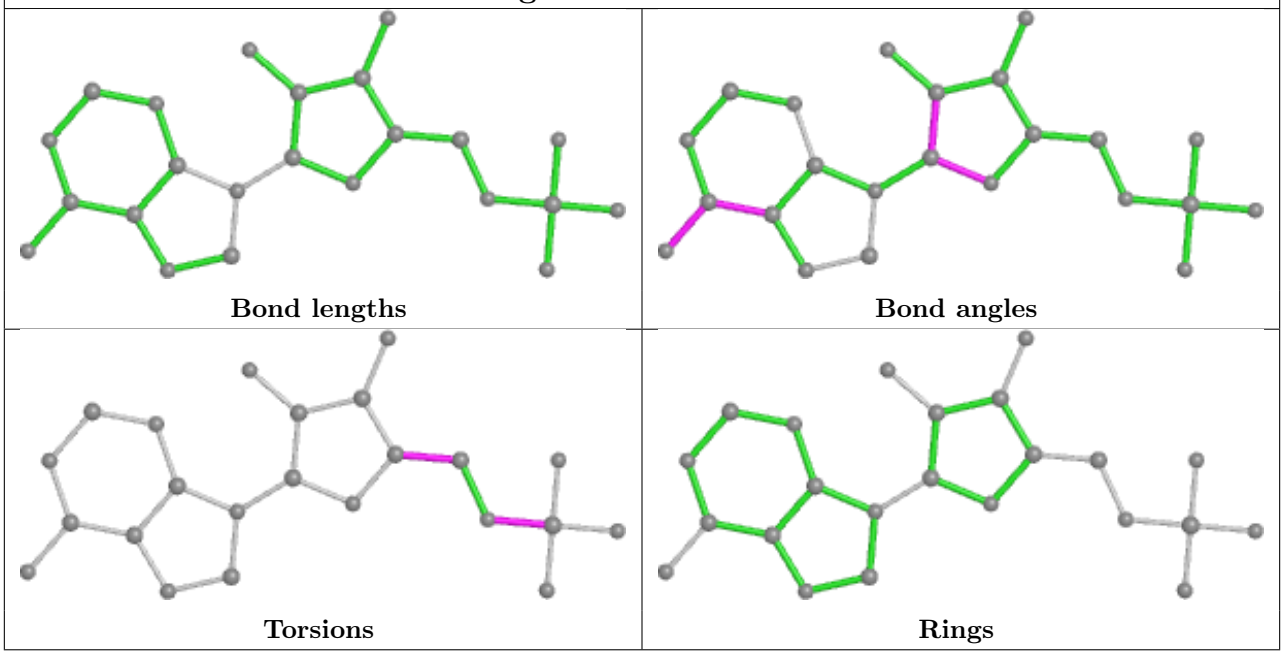
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	AMP	1	0

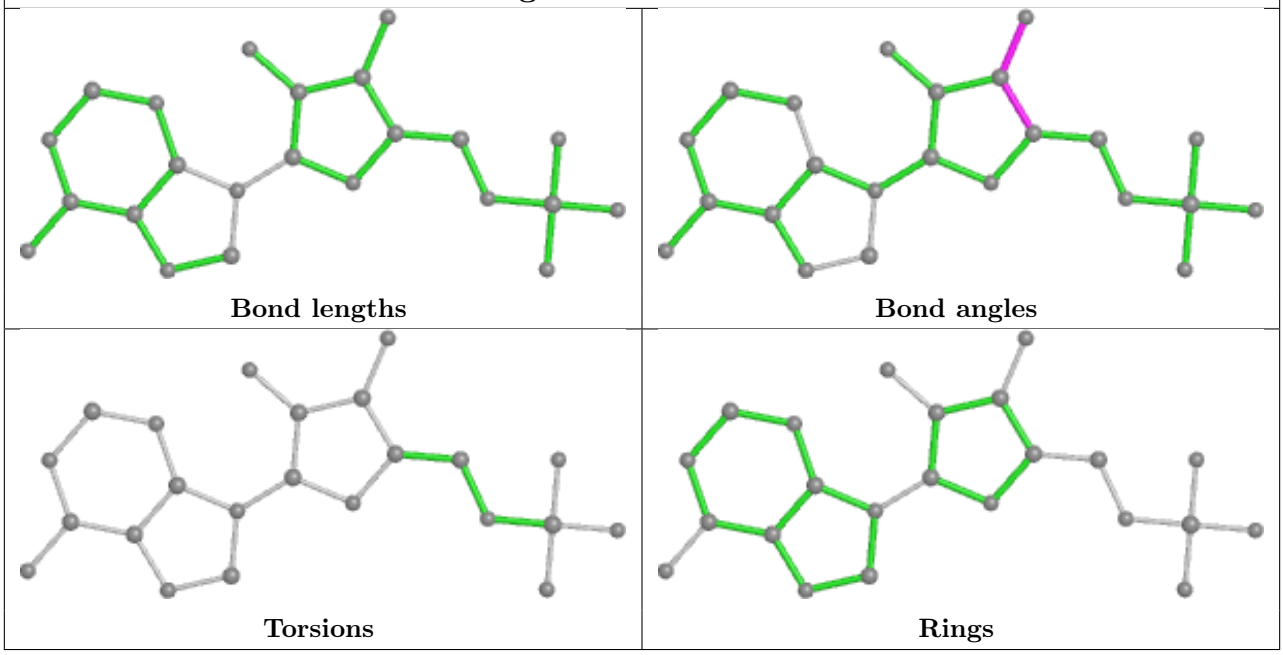
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

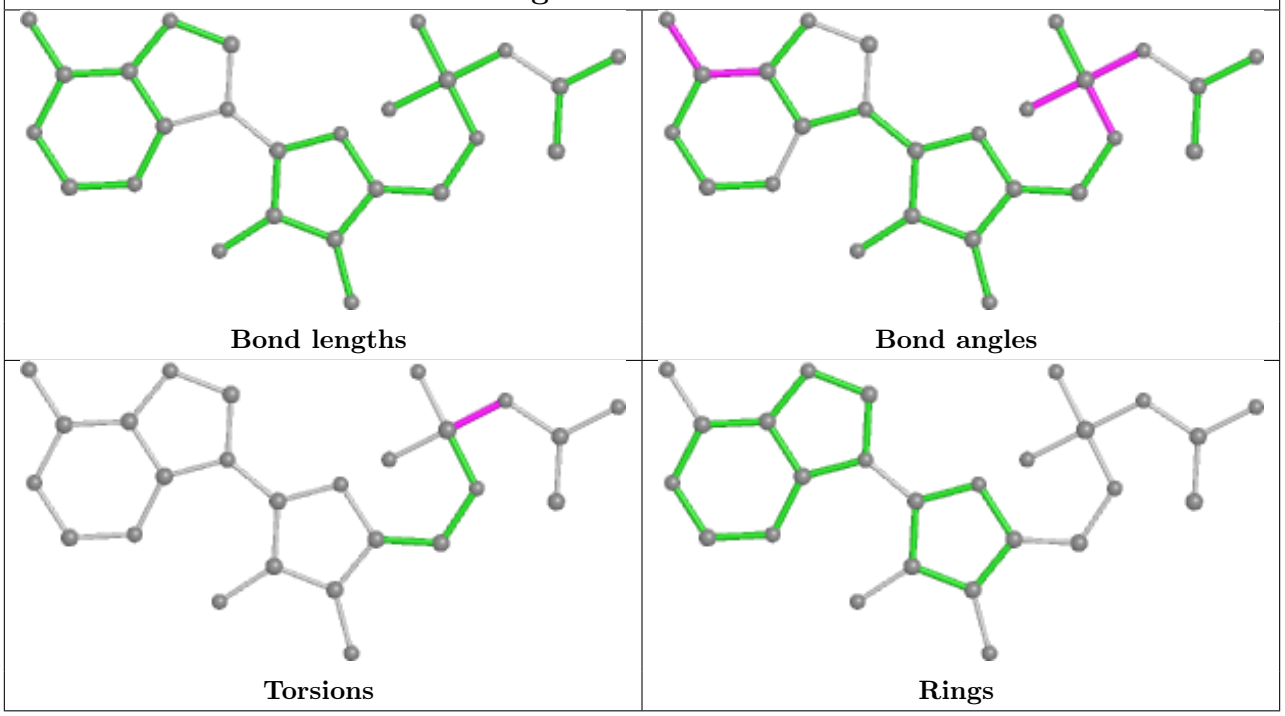
Ligand AMP A 601



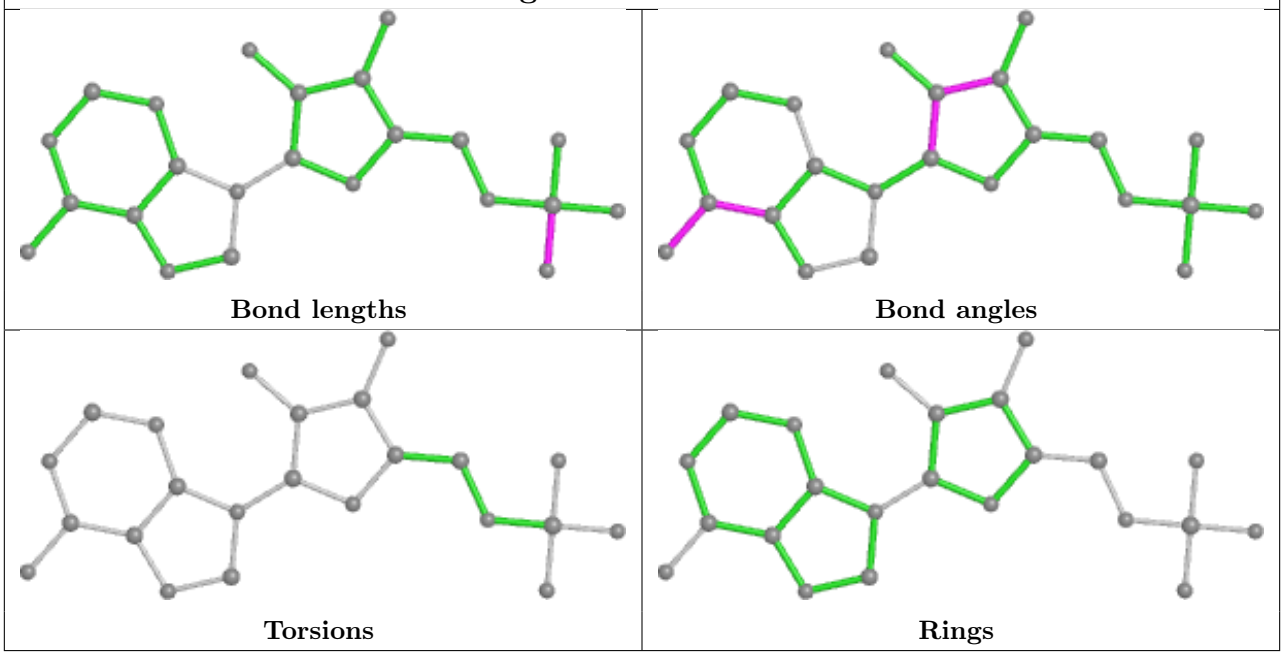
Ligand AMP D 601



Ligand 6R9 B 601



Ligand AMP C 601



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, 95^{th} 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%)	-0.20	8 (1%) 75 70	37, 50, 75, 112	0
1	B	561/570 (98%)	-0.03	15 (2%) 54 44	41, 57, 84, 100	0
1	C	554/570 (97%)	0.11	22 (3%) 38 28	46, 64, 97, 140	0
1	D	561/570 (98%)	0.01	18 (3%) 47 37	44, 61, 85, 104	0
All	All	2238/2280 (98%)	-0.03	63 (2%) 53 43	37, 58, 86, 140	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	ASN	5.2
1	B	290	VAL	4.7
1	A	352	GLY	4.6
1	B	565	GLN	4.5
1	A	192	SER	4.4
1	C	191	SER	4.1
1	C	192	SER	3.9
1	C	36	VAL	3.9
1	B	274	GLY	3.8
1	C	352	GLY	3.7
1	D	170	LEU	3.6
1	C	179	GLY	3.4
1	C	553	ARG	3.4
1	C	171	LYS	3.4
1	D	362	ASN	3.3
1	C	305	TRP	3.3
1	C	14	PHE	3.2
1	A	193	ASN	3.1
1	A	229	VAL	3.0
1	A	14	PHE	3.0
1	D	558	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	17	PHE	2.7
1	B	561	GLY	2.7
1	D	171	LYS	2.7
1	C	31	GLU	2.7
1	B	368	VAL	2.6
1	D	444	TYR	2.6
1	D	150	PRO	2.6
1	B	318	PHE	2.5
1	D	187	LEU	2.5
1	B	266	LEU	2.5
1	C	186	SER	2.5
1	D	76	ALA	2.5
1	D	149	LYS	2.4
1	B	287	LEU	2.4
1	D	274	GLY	2.4
1	B	560	LYS	2.3
1	C	298	PHE	2.3
1	C	243	SER	2.3
1	B	193	ASN	2.3
1	D	339	TRP	2.3
1	B	132	SER	2.2
1	C	557	LYS	2.2
1	C	190	GLU	2.2
1	C	564	GLY	2.2
1	C	387	ASP	2.2
1	A	389	GLY	2.2
1	C	445	PHE	2.2
1	B	148	LEU	2.1
1	D	361	GLY	2.1
1	C	204	VAL	2.1
1	C	367	LYS	2.1
1	D	148	LEU	2.1
1	B	264	SER	2.1
1	A	319	GLU	2.1
1	B	202	GLU	2.1
1	A	171	LYS	2.1
1	D	175	PHE	2.1
1	D	298	PHE	2.1
1	D	129	MET	2.1
1	D	115	HIS	2.1
1	D	57	LYS	2.0
1	B	157	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

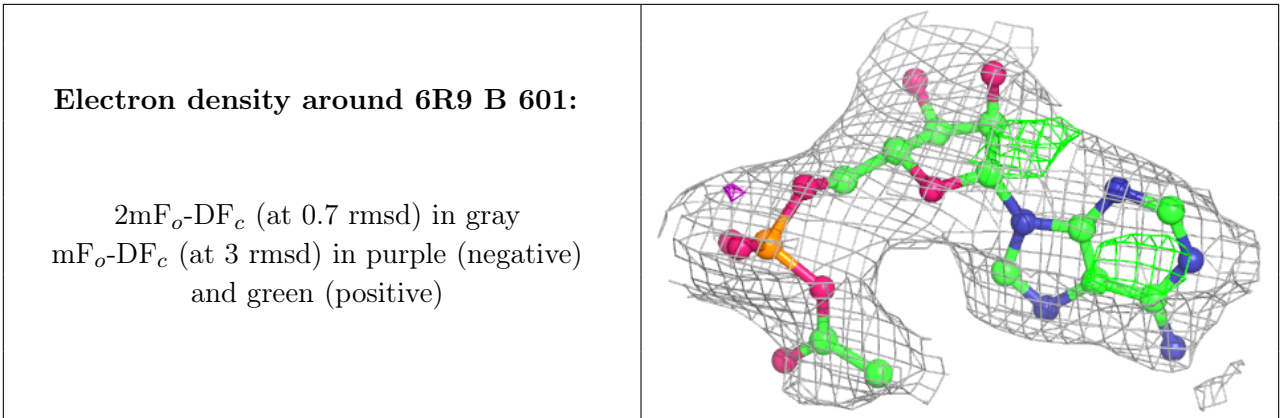
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

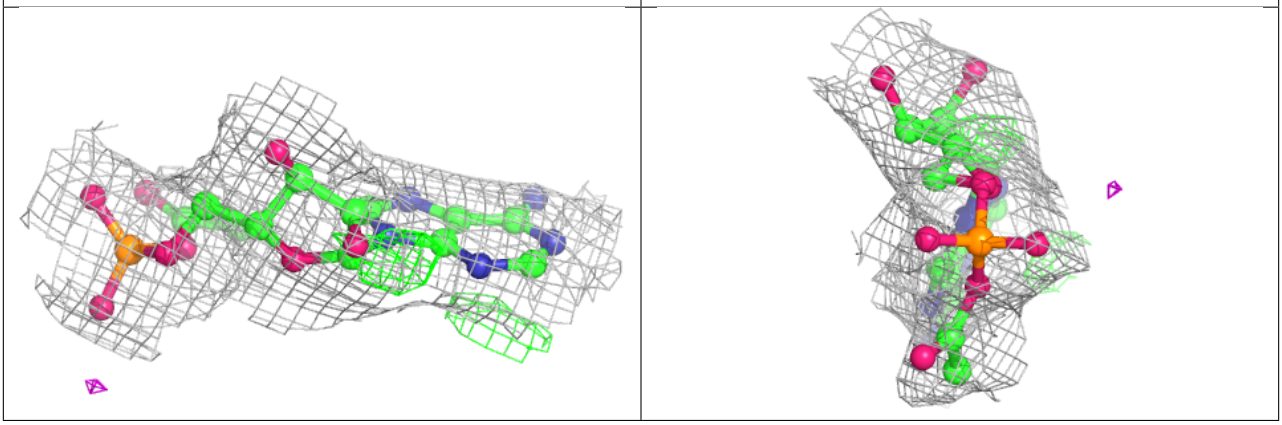
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	6R9	B	601	26/26	0.95	0.17	42,45,56,62	0
2	AMP	A	601	23/23	0.96	0.14	41,43,55,57	0
2	AMP	D	601	23/23	0.96	0.13	42,45,50,52	0
2	AMP	C	601	23/23	0.97	0.12	49,52,57,59	0

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 6R9 B 601:

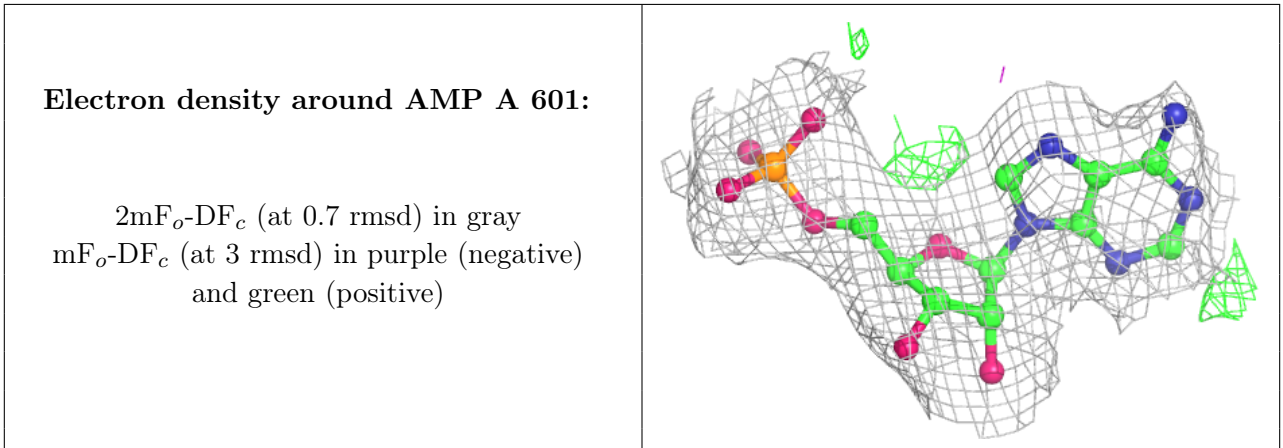
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

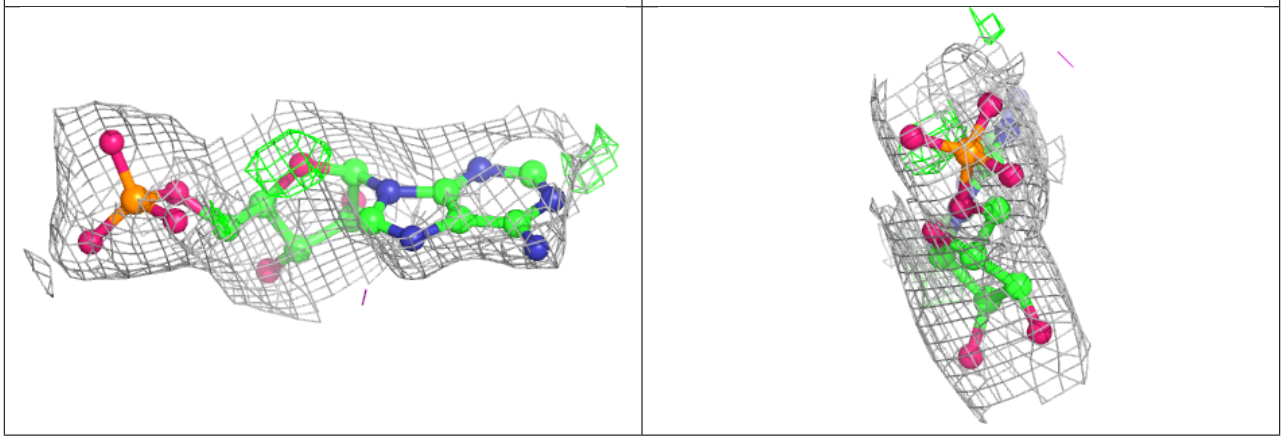




Electron density around AMP A 601:

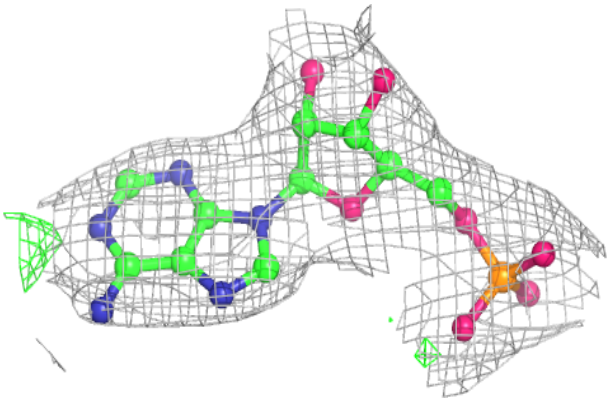
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

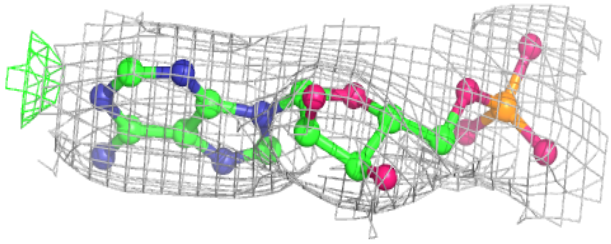


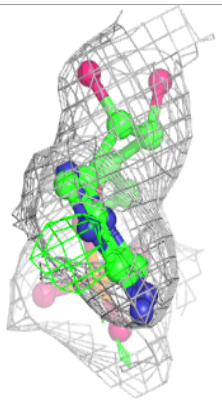


Electron density around AMP D 601:

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

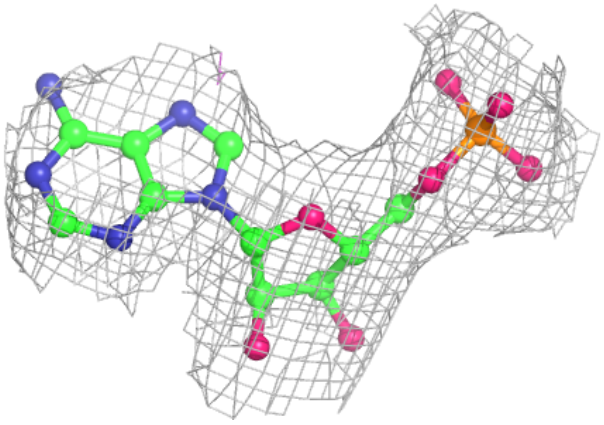


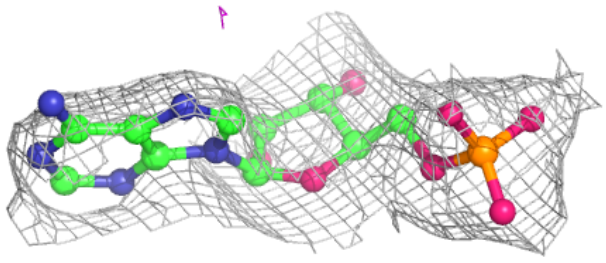


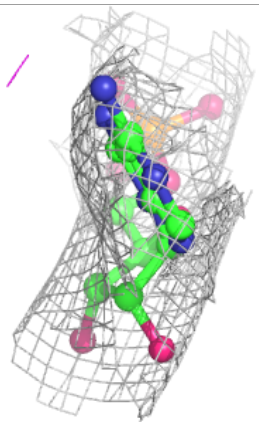


Electron density around AMP C 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.