



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:15 PM GMT

PDB ID : 4X4N  
Title : Crystal structure of the A.fulgidus CCA-adding enzyme in complex with a G70A arginyl-tRNA minihelix  
Authors : Kuhn, C.-D.; Joshua-Tor, L.  
Deposited on : 2014-12-03  
Resolution : 2.95 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

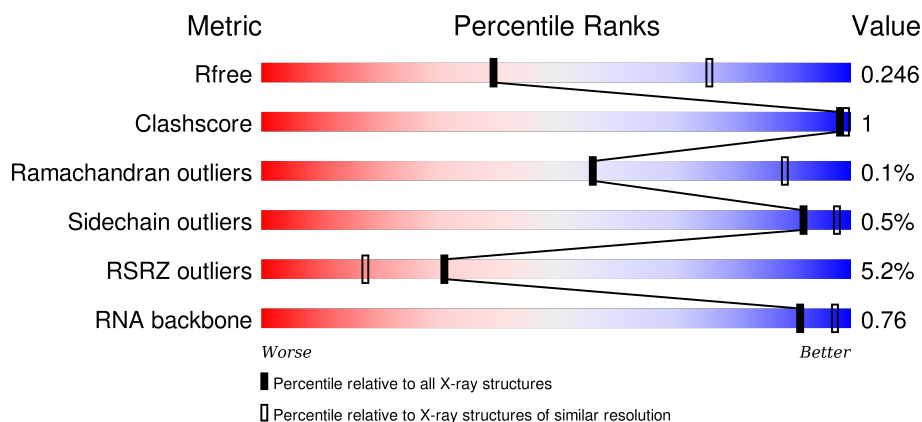
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	457	<div> <div>8%</div> <div>92%</div> <div>• •</div> </div>
1	C	457	<div> <div>8%</div> <div>93%</div> <div>• 5%</div> </div>
1	E	457	<div> <div>2%</div> <div>93%</div> <div>• •</div> </div>
1	F	457	<div> <div>2%</div> <div>93%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	34	<div><div></div><div>9%</div><div>82%</div><div>15%</div><div></div></div>
2	D	34	<div><div></div><div>3%</div><div>88%</div><div>9%</div><div></div></div>
2	G	34	<div><div></div><div>6%</div><div>50%</div><div>9%</div><div>41%</div><div></div></div>
3	I	2	<div><div></div><div>100%</div><div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32357 atoms, of which 15618 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 CCA-adding enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			7249	2333	3621	631	651	13			
1	C	436	Total	C	H	N	O	S	0	0	0
			7234	2328	3613	631	650	12			
1	E	437	Total	C	H	N	O	S	0	0	0
			7254	2333	3625	632	651	13			
1	F	437	Total	C	H	N	O	S	0	0	0
			7254	2333	3625	632	651	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	-	expression tag	UNP O28126
A	439	ASN	-	expression tag	UNP O28126
A	440	SER	-	expression tag	UNP O28126
A	441	SER	-	expression tag	UNP O28126
A	442	SER	-	expression tag	UNP O28126
A	443	VAL	-	expression tag	UNP O28126
A	444	ASP	-	expression tag	UNP O28126
A	445	LYS	-	expression tag	UNP O28126
A	446	LEU	-	expression tag	UNP O28126
A	447	ALA	-	expression tag	UNP O28126
A	448	ALA	-	expression tag	UNP O28126
A	449	ALA	-	expression tag	UNP O28126
A	450	LEU	-	expression tag	UNP O28126
A	451	GLU	-	expression tag	UNP O28126
A	452	HIS	-	expression tag	UNP O28126
A	453	HIS	-	expression tag	UNP O28126
A	454	HIS	-	expression tag	UNP O28126
A	455	HIS	-	expression tag	UNP O28126
A	456	HIS	-	expression tag	UNP O28126
A	457	HIS	-	expression tag	UNP O28126
C	438	SER	-	expression tag	UNP O28126

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Chain	Residue	Modelled	Actual	Comment	Reference
C	439	ASN	-	expression tag	UNP O28126
C	440	SER	-	expression tag	UNP O28126
C	441	SER	-	expression tag	UNP O28126
C	442	SER	-	expression tag	UNP O28126
C	443	VAL	-	expression tag	UNP O28126
C	444	ASP	-	expression tag	UNP O28126
C	445	LYS	-	expression tag	UNP O28126
C	446	LEU	-	expression tag	UNP O28126
C	447	ALA	-	expression tag	UNP O28126
C	448	ALA	-	expression tag	UNP O28126
C	449	ALA	-	expression tag	UNP O28126
C	450	LEU	-	expression tag	UNP O28126
C	451	GLU	-	expression tag	UNP O28126
C	452	HIS	-	expression tag	UNP O28126
C	453	HIS	-	expression tag	UNP O28126
C	454	HIS	-	expression tag	UNP O28126
C	455	HIS	-	expression tag	UNP O28126
C	456	HIS	-	expression tag	UNP O28126
C	457	HIS	-	expression tag	UNP O28126
E	438	SER	-	expression tag	UNP O28126
E	439	ASN	-	expression tag	UNP O28126
E	440	SER	-	expression tag	UNP O28126
E	441	SER	-	expression tag	UNP O28126
E	442	SER	-	expression tag	UNP O28126
E	443	VAL	-	expression tag	UNP O28126
E	444	ASP	-	expression tag	UNP O28126
E	445	LYS	-	expression tag	UNP O28126
E	446	LEU	-	expression tag	UNP O28126
E	447	ALA	-	expression tag	UNP O28126
E	448	ALA	-	expression tag	UNP O28126
E	449	ALA	-	expression tag	UNP O28126
E	450	LEU	-	expression tag	UNP O28126
E	451	GLU	-	expression tag	UNP O28126
E	452	HIS	-	expression tag	UNP O28126
E	453	HIS	-	expression tag	UNP O28126
E	454	HIS	-	expression tag	UNP O28126
E	455	HIS	-	expression tag	UNP O28126
E	456	HIS	-	expression tag	UNP O28126
E	457	HIS	-	expression tag	UNP O28126
F	438	SER	-	expression tag	UNP O28126
F	439	ASN	-	expression tag	UNP O28126
F	440	SER	-	expression tag	UNP O28126

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Chain	Residue	Modelled	Actual	Comment	Reference
F	441	SER	-	expression tag	UNP O28126
F	442	SER	-	expression tag	UNP O28126
F	443	VAL	-	expression tag	UNP O28126
F	444	ASP	-	expression tag	UNP O28126
F	445	LYS	-	expression tag	UNP O28126
F	446	LEU	-	expression tag	UNP O28126
F	447	ALA	-	expression tag	UNP O28126
F	448	ALA	-	expression tag	UNP O28126
F	449	ALA	-	expression tag	UNP O28126
F	450	LEU	-	expression tag	UNP O28126
F	451	GLU	-	expression tag	UNP O28126
F	452	HIS	-	expression tag	UNP O28126
F	453	HIS	-	expression tag	UNP O28126
F	454	HIS	-	expression tag	UNP O28126
F	455	HIS	-	expression tag	UNP O28126
F	456	HIS	-	expression tag	UNP O28126
F	457	HIS	-	expression tag	UNP O28126

- Molecule 2 is a RNA chain called G70A tRNA minihelix.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	18	Total	C	H	N	O	P	0	18	0
			1168	342	395	143	252	36			
2	B	32	Total	C	H	N	O	P	0	0	0
			1032	304	348	123	226	31			
2	D	31	Total	C	H	N	O	P	0	0	0
			999	294	337	118	220	30			

- Molecule 3 is a RNA chain called RNA (5'-D(P\*CP\*G)-3').

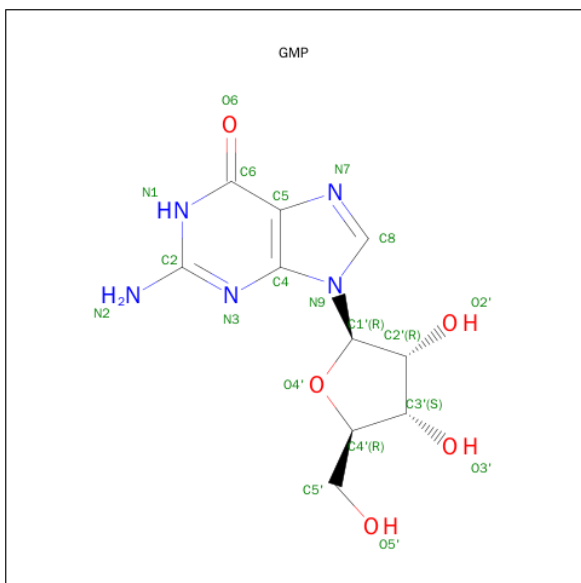
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	2	Total	C	H	N	O	P	0	0	0
			65	19	22	8	14	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



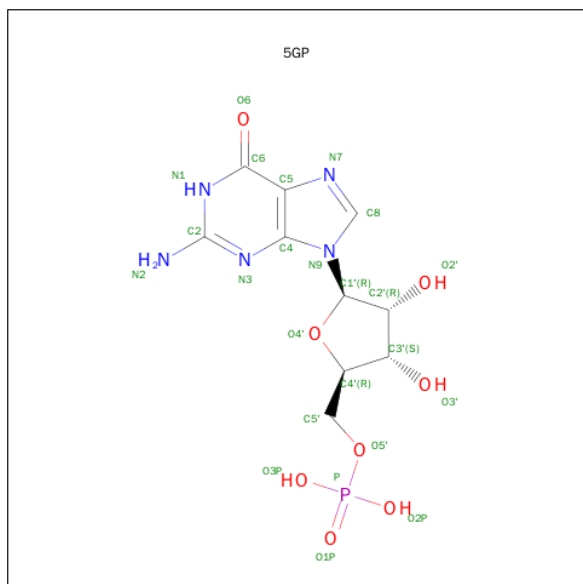
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GUANOSINE (three-letter code: GMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>5</sub>).



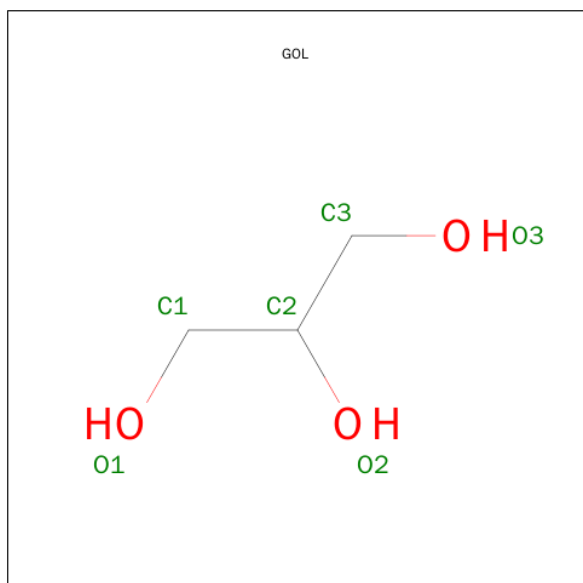
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	0	0
			32	10	12	5	5		

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	P	
			36	10	12	5	8	1	

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



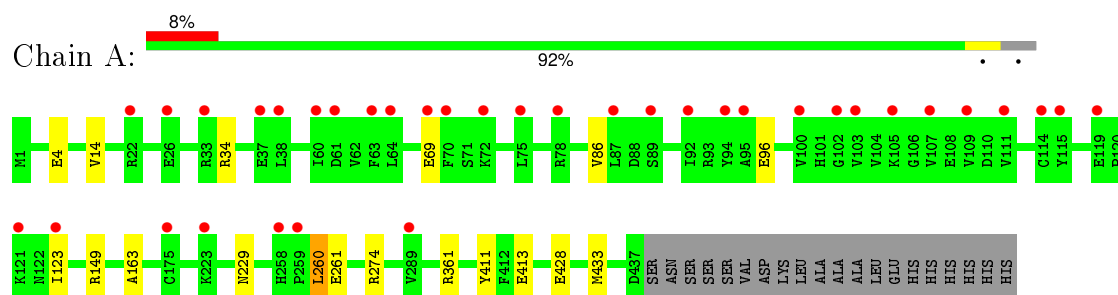


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			14	3	8	3		

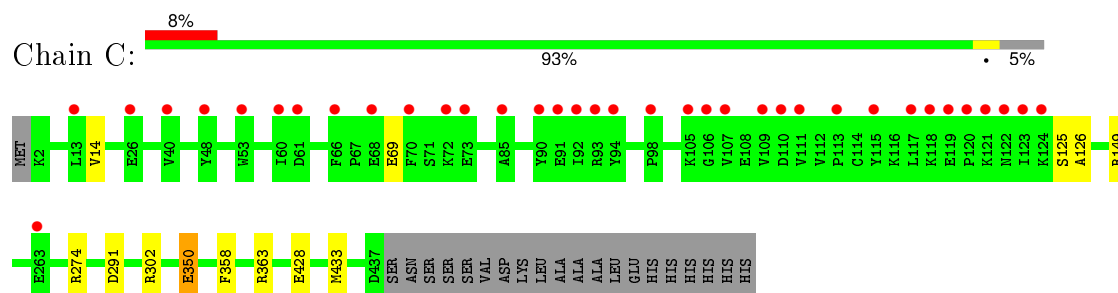
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

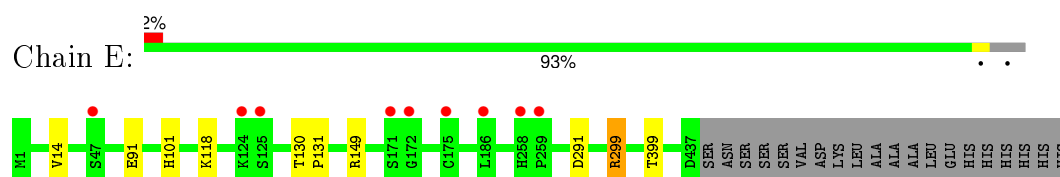
- Molecule 1: CCA-adding enzyme



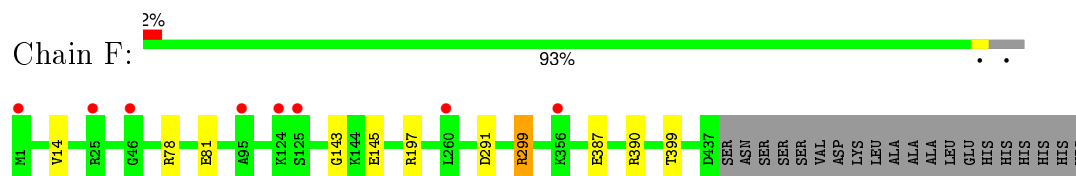
- Molecule 1: CCA-adding enzyme



- Molecule 1: CCA-adding enzyme



- Molecule 1: CCA-adding enzyme

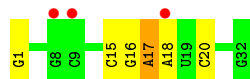
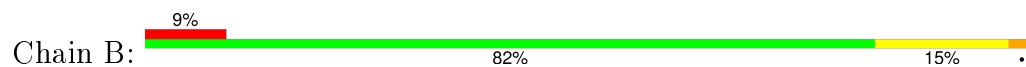


- Molecule 2: G70A tRNA minihelix

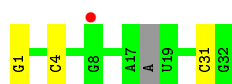
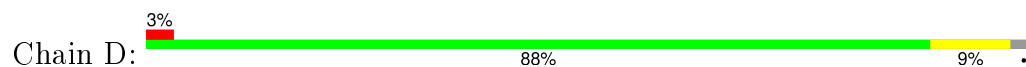




- Molecule 2: G70A tRNA minihelix



- Molecule 2: G70A tRNA minihelix



- Molecule 3: RNA (5'-D(P\*CP\*G)-3')



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.42Å 84.69Å 135.56Å 90.00° 103.14° 90.00°	Depositor
Resolution (Å)	29.89 – 2.95 29.88 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.89-2.95) 99.1 (29.88-2.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.191 , 0.249 0.199 , 0.246	Depositor DCC
$R_{free}$ test set	2669 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53316 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 5GP, GOL, GMP, SO4

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	0.22	0/3711	0.36	0/4985
1	C	0.22	0/3704	0.36	0/4977
1	E	0.23	0/3712	0.37	0/4987
1	F	0.23	0/3712	0.38	0/4987
2	B	0.42	1/760 (0.1%)	0.66	0/1180
2	D	0.42	1/734 (0.1%)	0.66	0/1137
2	G	0.14	0/855	0.66	0/1316
3	I	0.14	0/47	0.63	0/71
All	All	0.24	2/17235 (0.0%)	0.43	0/23640

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	G	OP3-P	-10.62	1.48	1.61
2	D	1	G	OP3-P	-10.55	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	3621	3629	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3621	3613	3621	9	0
1	E	3629	3625	3633	6	0
1	F	3629	3625	3633	6	0
2	B	684	348	350	2	0
2	D	662	337	340	2	0
2	G	773	395	399	3	0
3	I	43	22	23	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	B	20	12	13	0	0
6	B	24	12	12	0	0
7	D	6	8	8	0	0
All	All	16739	15618	15661	30	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 1.

All (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:NH2	1:A:433:MET:O	2.22	0.72
1:C:274:ARG:NH2	1:C:433:MET:O	2.27	0.68
1:A:361:ARG:NH2	2:B:15:C:OP2	2.30	0.64
1:F:299:ARG:NH1	1:F:399:THR:O	2.31	0.62
1:F:78:ARG:NH1	1:F:81:GLU:OE1	2.32	0.62
1:E:299:ARG:NH1	1:E:399:THR:O	2.33	0.62
2:G:9[B]:C:O2'	1:E:291:ASP:OD1	2.21	0.58
1:C:428:GLU:N	1:C:428:GLU:OE1	2.37	0.57
2:G:31[A]:C:O2'	1:E:291:ASP:OD1	2.21	0.57
1:A:69:GLU:OE1	1:A:69:GLU:N	2.38	0.57
2:G:8[A]:G:O2'	1:F:291:ASP:OD1	2.23	0.57
1:C:358:PHE:O	1:C:363:ARG:NH2	2.38	0.55
1:A:163:ALA:O	1:A:229:ASN:ND2	2.39	0.53
1:E:91:GLU:N	1:E:101:HIS:O	2.42	0.52
1:C:125:SER:OG	1:C:126:ALA:N	2.44	0.51
1:C:302:ARG:NH2	2:D:4:C:OP1	2.44	0.51
1:F:143:GLY:N	1:F:145:GLU:OE1	2.44	0.48
1:E:14:VAL:CG1	1:E:149:ARG:HB3	2.43	0.47
1:C:69:GLU:N	1:C:69:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASP:OD1	2:D:31:C:O2'	2.32	0.47
1:A:14:VAL:CG1	1:A:149:ARG:HB3	2.44	0.46
1:A:411:TYR:OH	1:A:413:GLU:OE2	2.32	0.46
1:A:428:GLU:N	1:A:428:GLU:OE1	2.49	0.45
1:A:4:GLU:N	1:A:4:GLU:OE1	2.49	0.45
2:B:16:G:H2'	2:B:17:A:H5'	1.99	0.44
1:C:350:GLU:OE1	1:F:197:ARG:NH2	2.49	0.43
1:F:387:GLU:OE2	1:F:390:ARG:NH1	2.52	0.43
1:E:130:THR:HB	1:E:131:PRO:HD3	2.01	0.43
1:A:34:ARG:NH1	1:A:86:VAL:O	2.45	0.43
1:C:14:VAL:CG1	1:C:149:ARG:HB3	2.49	0.42

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	435/457 (95%)	405 (93%)	28 (6%)	2 (0%)	34	74
1	C	434/457 (95%)	421 (97%)	13 (3%)	0	100	100
1	E	435/457 (95%)	416 (96%)	19 (4%)	0	100	100
1	F	435/457 (95%)	421 (97%)	14 (3%)	0	100	100
All	All	1739/1828 (95%)	1663 (96%)	74 (4%)	2 (0%)	56	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	LEU
1	A	123	ILE

### 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	386/404 (96%)	383 (99%)	3 (1%)	86	95
1	C	386/404 (96%)	385 (100%)	1 (0%)	94	98
1	E	387/404 (96%)	385 (100%)	2 (0%)	92	97
1	F	387/404 (96%)	385 (100%)	2 (0%)	92	97
All	All	1546/1616 (96%)	1538 (100%)	8 (0%)	92	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLU
1	A	260	LEU
1	A	261	GLU
1	C	350	GLU
1	E	118	LYS
1	E	299	ARG
1	F	14	VAL
1	F	299	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	30/34 (88%)	3 (10%)	0
2	D	28/34 (82%)	0	0
2	G	1/34 (2%)	0	0
3	I	1/2 (50%)	0	0
All	All	60/104 (57%)	3 (5%)	0

All (3) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
2	B	17	A
2	B	18	A
2	B	20	C

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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
4	SO4	A	501	-	4,4,4	0.21	0	6,6,6	0.09	0
5	GMP	B	101	-	17,22,22	3.27	6 (35%)	17,33,33	1.24	3 (17%)
6	5GP	B	102	-	21,26,26	0.96	1 (4%)	23,40,40	1.05	1 (4%)
4	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.09	0
7	GOL	D	101	-	5,5,5	0.34	0	5,5,5	0.21	0
4	SO4	E	501	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	F	501	-	4,4,4	0.22	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	501	-	-	0/0/0/0	0/0/0/0
5	GMP	B	101	-	-	0/2/22/22	0/3/3/3
6	5GP	B	102	-	-	0/6/26/26	0/3/3/3
4	SO4	C	501	-	-	0/0/0/0	0/0/0/0
7	GOL	D	101	-	-	0/4/4/4	0/0/0/0
4	SO4	E	501	-	-	0/0/0/0	0/0/0/0
4	SO4	F	501	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	101	GMP	C6-N1	2.19	1.39	1.36
6	B	102	5GP	C2-N2	2.42	1.35	1.32
5	B	101	GMP	C6-C5	2.97	1.46	1.41
5	B	101	GMP	C2-N3	3.20	1.37	1.33
5	B	101	GMP	C2-N1	5.30	1.44	1.36
5	B	101	GMP	C4-N3	7.75	1.47	1.35
5	B	101	GMP	C2-N2	8.09	1.44	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	101	GMP	C4-C5-N7	-2.44	107.23	109.48
6	B	102	5GP	C1'-N9-C4	-2.36	123.38	126.94
5	B	101	GMP	N1-C2-N3	-2.28	118.73	121.79
5	B	101	GMP	N2-C2-N1	3.49	121.61	117.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/457 (95%)	0.44	36 (8%) 14 7	12, 40, 143, 158	0
1	C	436/457 (95%)	0.53	36 (8%) 14 7	10, 41, 132, 147	0
1	E	437/457 (95%)	0.08	9 (2%) 67 46	9, 30, 64, 98	0
1	F	437/457 (95%)	0.07	8 (1%) 71 51	10, 26, 64, 101	0
2	B	34/34 (100%)	0.75	3 (8%) 12 6	45, 72, 107, 182	0
2	D	33/34 (97%)	0.61	1 (3%) 54 33	33, 56, 88, 88	0
2	G	20/34 (58%)	0.53	2 (10%) 9 5	33, 35, 61, 61	4 (20%)
3	I	2/2 (100%)	1.65	0 100 100	57, 57, 57, 78	0
All	All	1836/1932 (95%)	0.30	95 (5%) 31 17	9, 34, 128, 182	4 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	TYR	8.1
1	C	122	ASN	6.4
1	C	73	GLU	5.8
1	C	94	TYR	5.1
2	B	18	A	4.1
1	A	121	LYS	4.0
1	C	98	PRO	4.0
1	C	70	PHE	3.9
1	C	92	ILE	3.9
1	A	258	HIS	3.8
1	A	105	LYS	3.7
1	C	123	ILE	3.7
1	C	105	LYS	3.6
1	F	260	LEU	3.6
1	A	103	VAL	3.5
1	A	89	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	115	TYR	3.3
1	A	61	ASP	3.3
1	C	121	LYS	3.3
1	C	61	ASP	3.3
1	C	72	LYS	3.2
1	E	175	CYS	3.2
1	C	107	VAL	3.2
1	C	117	LEU	3.2
1	C	115	TYR	3.1
1	A	259	PRO	3.1
1	C	40	VAL	3.0
1	A	72	LYS	3.0
1	C	110	ASP	3.0
1	E	124	LYS	2.9
1	C	85	ALA	2.9
1	C	60	ILE	2.9
1	A	69	GLU	2.9
1	C	91	GLU	2.9
1	C	124	LYS	2.8
2	B	8	G	2.8
1	C	118	LYS	2.8
1	C	111	VAL	2.7
1	C	109	VAL	2.7
1	A	60	ILE	2.7
1	E	47	SER	2.7
1	A	22	ARG	2.6
1	A	175	CYS	2.6
1	A	87	LEU	2.6
1	C	119	GLU	2.6
1	C	13	LEU	2.6
1	E	259	PRO	2.6
1	A	100	VAL	2.5
1	A	114	CYS	2.5
2	G	1[A]	G	2.5
1	A	107	VAL	2.4
1	A	37	GLU	2.4
1	A	78	ARG	2.4
1	C	263	GLU	2.4
1	C	66	PHE	2.4
1	E	258	HIS	2.3
1	A	95	ALA	2.3
2	G	23[A]	G	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	106	GLY	2.3
1	A	92	ILE	2.3
1	E	171	SER	2.3
1	A	289	VAL	2.3
1	A	111	VAL	2.3
1	F	95	ALA	2.2
1	C	68	GLU	2.2
1	A	26	GLU	2.2
1	A	109	VAL	2.2
2	B	9	C	2.2
1	A	119	GLU	2.2
1	F	356	LYS	2.2
1	F	1	MET	2.2
1	A	123	ILE	2.2
1	F	25	ARG	2.2
1	C	26	GLU	2.2
1	C	120	PRO	2.2
1	A	102	GLY	2.2
2	D	8	G	2.2
1	E	125	SER	2.1
1	A	63	PHE	2.1
1	C	53	TRP	2.1
1	C	93	ARG	2.1
1	A	33	ARG	2.1
1	C	113	PRO	2.1
1	A	38	LEU	2.1
1	A	64	LEU	2.1
1	E	172	GLY	2.1
1	A	70	PHE	2.1
1	F	124	LYS	2.1
1	A	75	LEU	2.1
1	E	186	LEU	2.0
1	A	223	LYS	2.0
1	C	48	TYR	2.0
1	C	90	TYR	2.0
1	F	46	GLY	2.0
1	F	125	SER	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	5GP	B	102	24/24	0.74	0.32	0.72	48,85,106,118	0
4	SO4	A	501	5/5	0.90	0.29	0.65	53,56,83,87	0
5	GMP	B	101	20/20	0.86	0.26	0.15	45,65,87,89	0
4	SO4	F	501	5/5	0.97	0.21	-0.06	31,40,53,59	0
4	SO4	E	501	5/5	0.93	0.25	-0.26	43,52,73,73	0
4	SO4	C	501	5/5	0.88	0.23	-0.52	72,77,89,95	0
7	GOL	D	101	6/6	0.71	0.22	-	59,74,89,91	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.