Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:26 am BST

PDB ID	:	4X4P
Title	:	Crystal structure of the A.fulgidus CCA-adding enzyme in complex with a G70A arginyl-tRNA minihelix ending in CCAC
Authors	:	Kuhn, C.-D.; Joshua-Tor, L.
Deposited on	:	2014-12-03
Resolution	:	3.00 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 following versions of software and data (see references ①) were used in the production of this report:

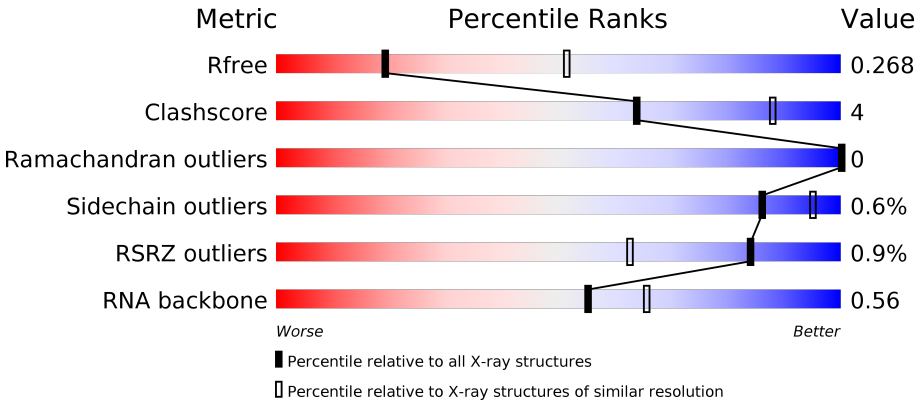
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



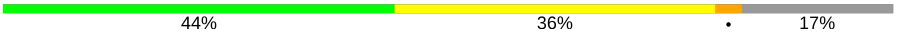
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	457	% 82% 13% .
1	C	457	% 85% 10% 5%
1	E	457	% 85% 9% 6%
1	G	457	% 82% 11% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	36	
2	D	36	
2	F	36	
2	H	36	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32633 atoms, of which 15667 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
			7270	2333	3641	632	651	13			
1	C	434	Total	C	H	N	O	S	0	0	0
			7212	2317	3609	628	646	12			
1	E	428	Total	C	H	N	O	S	0	0	0
			7102	2279	3556	619	636	12			
1	G	428	Total	C	H	N	O	S	0	0	0
			7102	2284	3548	619	639	12			

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

Continued on next page...

Continued from previous page...

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
G	438	SER	-	expression tag	UNP O28126
G	439	ASN	-	expression tag	UNP O28126
G	440	SER	-	expression tag	UNP O28126

Continued on next page...

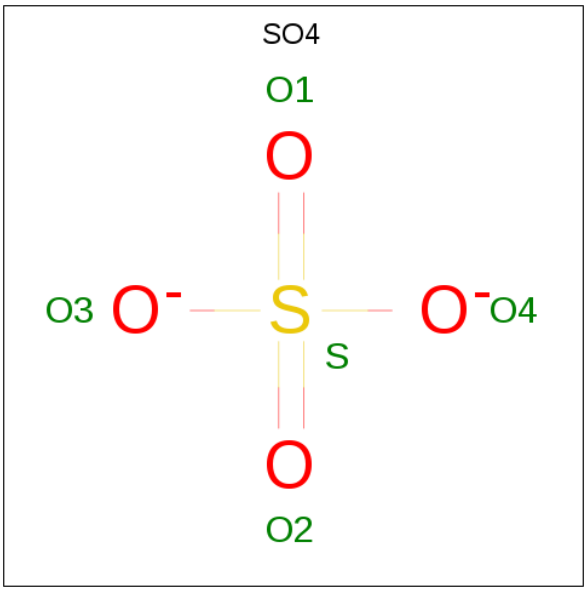
Continued from previous page...

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	36	Total	C	H	N	O	P	0	0	0
			1157	341	390	137	253	36			
2	D	30	Total	C	H	N	O	P	0	0	0
			966	284	326	114	212	30			
2	F	27	Total	C	H	N	O	P	0	0	0
			873	257	293	105	191	27			
2	H	28	Total	C	H	N	O	P	0	0	0
			901	265	304	106	198	28			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



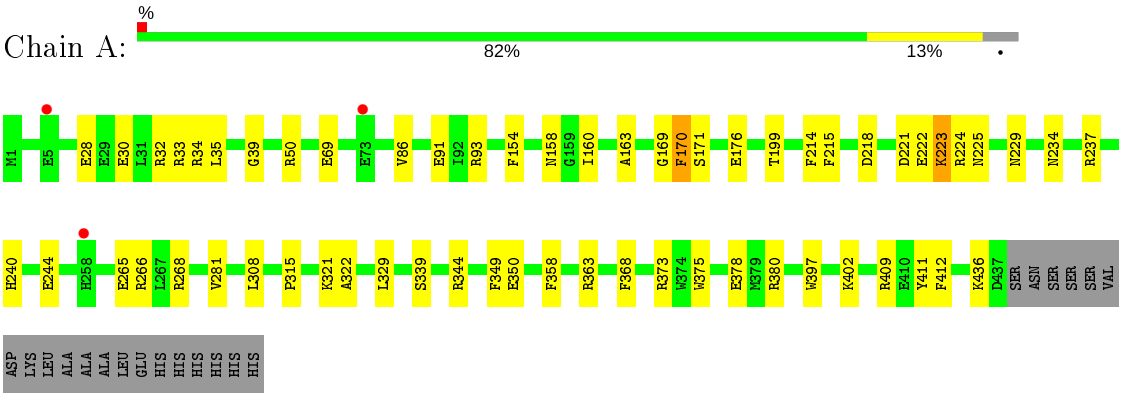
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0

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 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.

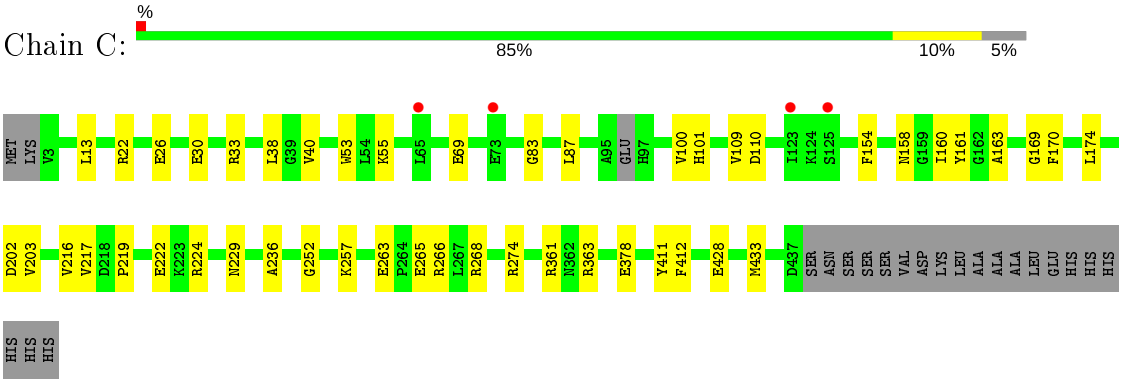
- Molecule 1: CCA-adding enzyme

Chain A:



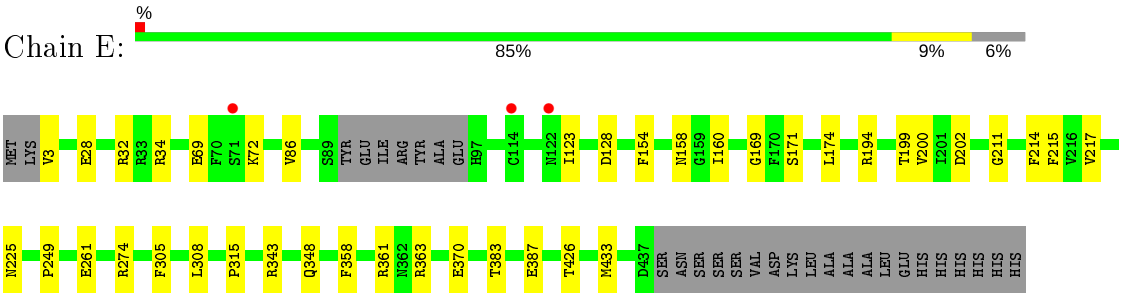
- Molecule 1: CCA-adding enzyme

Chain C:



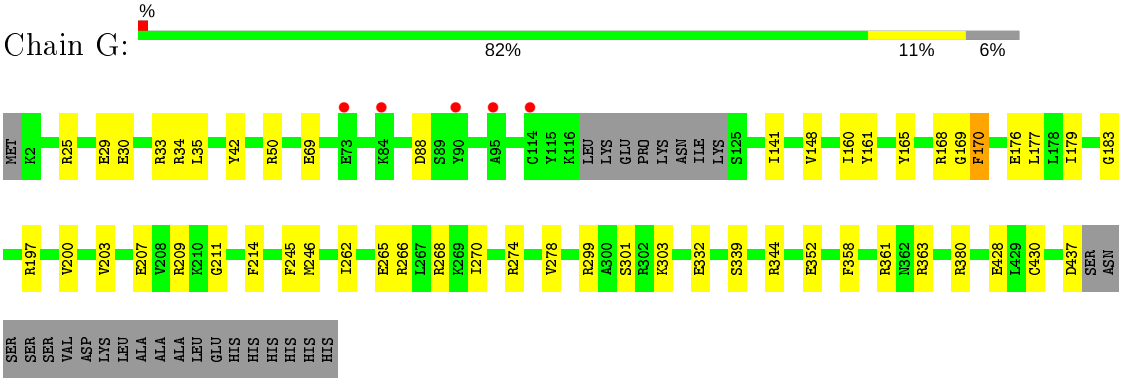
- Molecule 1: CCA-adding enzyme

Chain E:



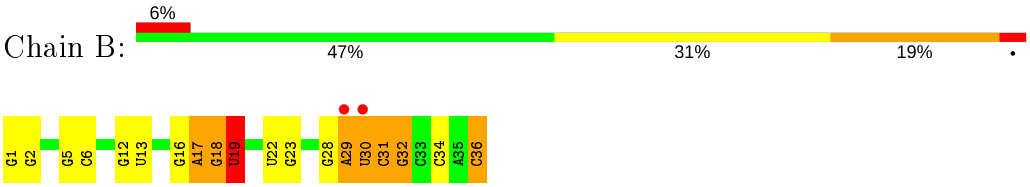
- Molecule 1: CCA-adding enzyme

Chain G:



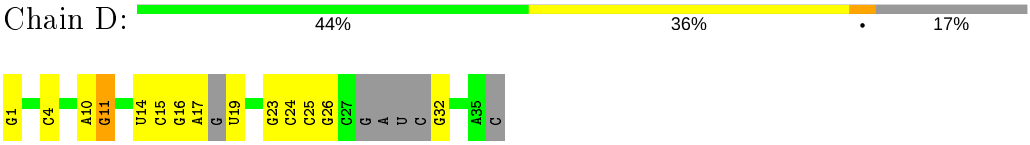
• Molecule 2: G70A tRNA minihelix ending in CCAC

Chain B:



• Molecule 2: G70A tRNA minihelix ending in CCAC

Chain D:

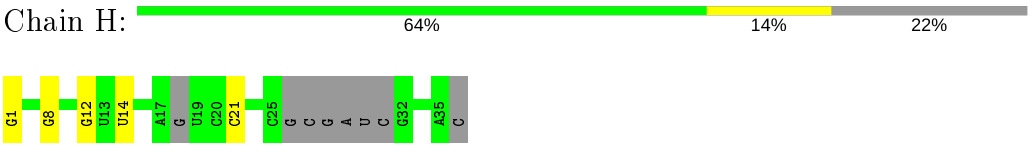


• Molecule 2: G70A tRNA minihelix ending in CCAC

Chain F:

• Molecule 2: G70A tRNA minihelix ending in CCAC

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.11Å 58.11Å 217.81Å 85.20° 87.98° 89.81°	Depositor
Resolution (Å)	29.58 – 3.00 29.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	85.6 (29.58-3.00) 87.5 (29.58-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.224 , 0.274 0.220 , 0.268	Depositor DCC
R_{free} test set	1859 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.060 for -k,-h,-l	Xtriage
Reported twinning fraction	0.130 for -k,-h,-l	Depositor
Outliers	0 of 49715 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	32633	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.75% 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: 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	0.40	0/3712	0.56	0/4987
1	C	0.40	0/3685	0.57	0/4951
1	E	0.42	0/3626	0.57	0/4871
1	G	0.41	0/3635	0.58	0/4884
2	B	0.42	0/855	0.96	2/1331 (0.2%)
2	D	0.53	1/711 (0.1%)	0.88	1/1100 (0.1%)
2	F	0.53	1/646 (0.2%)	0.83	0/1002
2	H	0.55	1/663 (0.2%)	0.90	1/1025 (0.1%)
All	All	0.43	3/17533 (0.0%)	0.64	4/24151 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	G	OP3-P	-10.46	1.48	1.61
2	D	1	G	OP3-P	-10.41	1.48	1.61
2	F	1	G	OP3-P	-10.13	1.49	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	G	OP1-P-O3'	5.67	117.66	105.20
2	D	1	G	OP1-P-O3'	5.39	117.07	105.20
2	B	19	U	C2-N1-C1'	5.16	123.89	117.70
2	H	1	G	OP1-P-O3'	5.04	116.28	105.20

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	3629	3641	3633	35	0
1	C	3603	3609	3601	26	0
1	E	3546	3556	3548	25	0
1	G	3554	3548	3540	29	0
2	B	767	390	392	16	0
2	D	640	326	329	9	0
2	F	580	293	295	3	0
2	H	597	304	307	2	0
3	A	25	0	0	2	0
3	C	5	0	0	0	0
3	E	10	0	0	1	0
3	G	10	0	0	0	0
All	All	16966	15667	15645	136	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 4.

All (136) 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:E:194:ARG:NH1	1:G:352:GLU:OE2	2.12	0.82
1:A:358:PHE:O	1:A:363:ARG:NH2	2.14	0.79
1:C:154:PHE:O	1:C:158:ASN:ND2	2.16	0.78
1:E:358:PHE:O	1:E:363:ARG:NH2	2.18	0.77
1:A:34:ARG:NH1	1:A:86:VAL:O	2.19	0.76
1:A:30:GLU:OE2	1:A:33:ARG:NH1	2.22	0.73
1:C:30:GLU:OE2	1:C:33:ARG:NH1	2.24	0.70
2:B:31:C:H3'	2:B:32:G:C5'	2.22	0.70
2:B:29:A:O2'	2:B:30:U:OP1	2.10	0.69
1:E:28:GLU:OE2	1:E:32:ARG:NH1	2.26	0.69
1:G:207:GLU:OE1	1:G:209:ARG:NH1	2.26	0.69
1:G:34:ARG:NH1	1:G:88:ASP:OD1	2.27	0.67
1:A:266:ARG:NH2	1:A:436:LYS:O	2.29	0.65
2:B:29:A:H3'	2:B:30:U:H5'	1.77	0.65
1:C:69:GLU:OE1	1:C:69:GLU:N	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:O	2:B:31:C:N4	2.30	0.64
1:A:50:ARG:NH1	1:A:176:GLU:OE2	2.31	0.63
1:C:252:GLY:O	1:C:257:LYS:NZ	2.28	0.62
1:A:344:ARG:NH1	1:A:378:GLU:OE1	2.33	0.61
1:E:69:GLU:OE1	1:E:69:GLU:N	2.34	0.60
2:B:18:G:O2'	2:B:19:U:OP1	2.20	0.59
1:G:69:GLU:OE1	1:G:69:GLU:N	2.36	0.59
1:C:163:ALA:O	1:C:229:ASN:ND2	2.35	0.58
1:A:339:SER:O	1:A:380:ARG:NH1	2.35	0.58
1:G:50:ARG:NH1	1:G:176:GLU:OE1	2.37	0.58
1:A:69:GLU:OE1	1:A:69:GLU:N	2.36	0.57
1:E:34:ARG:NH1	1:E:86:VAL:O	2.35	0.57
1:C:87:LEU:HD11	1:C:109:VAL:HB	1.87	0.56
1:E:160:ILE:O	1:E:169:GLY:HA3	2.06	0.56
1:A:154:PHE:O	1:A:158:ASN:ND2	2.35	0.56
1:E:361:ARG:NH2	2:F:15:C:OP2	2.40	0.53
1:E:308:LEU:HB3	1:E:315:PRO:HG3	1.89	0.53
1:C:274:ARG:NH2	1:C:433:MET:O	2.41	0.53
1:E:305:PHE:CE2	1:E:315:PRO:HB2	2.44	0.52
1:C:202:ASP:HA	1:C:217:VAL:CG1	2.39	0.52
1:A:35:LEU:O	1:A:39:GLY:N	2.43	0.51
1:C:363:ARG:NH1	1:C:378:GLU:OE2	2.44	0.51
1:C:101:HIS:ND1	1:C:110:ASP:OD1	2.38	0.51
1:G:358:PHE:O	1:G:363:ARG:NH2	2.43	0.50
1:A:373:ARG:NH1	3:A:504:SO4:O1	2.43	0.50
1:E:154:PHE:O	1:E:158:ASN:ND2	2.45	0.50
1:E:308:LEU:CB	1:E:315:PRO:HG3	2.43	0.49
1:E:348:GLN:NE2	3:E:502:SO4:O2	2.45	0.49
1:A:224:ARG:NH2	2:B:34:C:OP2	2.46	0.49
2:B:31:C:H3'	2:B:32:G:H5"	1.92	0.49
2:D:17:A:H2'	2:D:19:U:C6	2.48	0.49
2:B:18:G:HO2'	2:B:19:U:P	2.36	0.48
1:C:203:VAL:HB	1:C:219:PRO:HG3	1.95	0.48
1:C:22:ARG:NH1	1:C:26:GLU:OE2	2.46	0.48
1:C:428:GLU:OE1	1:C:428:GLU:N	2.44	0.48
1:E:361:ARG:NH2	2:F:14:U:OP1	2.46	0.48
3:A:505:SO4:O4	2:B:36:C:N4	2.47	0.48
1:A:308:LEU:CB	1:A:315:PRO:HG3	2.44	0.47
1:G:262:ILE:HD13	1:G:430:CYS:SG	2.54	0.47
1:G:30:GLU:HA	1:G:33:ARG:NH1	2.30	0.47
1:E:202:ASP:HA	1:E:217:VAL:CG1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:C:N4	2:D:16:G:C6	2.83	0.47
1:G:339:SER:O	1:G:380:ARG:NH1	2.46	0.47
1:E:343:ARG:NH2	1:E:370:GLU:OE2	2.48	0.47
2:D:23:G:C6	2:D:24:C:C4	3.03	0.46
1:A:199:THR:O	1:A:214:PHE:HA	2.16	0.46
1:E:215:PHE:HA	1:E:225:ASN:ND2	2.31	0.46
1:A:397:TRP:CZ2	1:A:409:ARG:HD3	2.49	0.46
1:E:123:ILE:HG23	1:E:128:ASP:HB2	1.98	0.46
1:G:177:LEU:HD13	1:G:203:VAL:HG21	1.97	0.46
1:A:28:GLU:OE2	1:A:32:ARG:NH1	2.49	0.45
1:G:30:GLU:OE2	1:G:33:ARG:NH1	2.44	0.45
1:A:281:VAL:HB	1:A:329:LEU:HB2	1.97	0.45
1:A:234:ASN:OD1	1:A:237:ARG:NH1	2.49	0.45
2:F:13:U:H2'	2:F:14:U:O4'	2.17	0.45
1:A:163:ALA:O	1:A:229:ASN:ND2	2.40	0.45
2:H:12:G:C2	2:H:21:C:C2	3.05	0.45
1:A:402:LYS:NZ	2:B:2:G:OP1	2.27	0.45
2:D:10:A:C6	2:D:23:G:N1	2.85	0.45
1:C:265:GLU:OE1	1:C:268:ARG:NH2	2.45	0.44
1:A:163:ALA:HB2	1:A:171:SER:HB3	1.99	0.44
2:B:5:G:H2'	2:B:6:C:O4'	2.17	0.44
1:E:383:THR:N	1:E:387:GLU:OE1	2.44	0.44
1:G:428:GLU:OE1	1:G:428:GLU:N	2.50	0.44
1:A:160:ILE:O	1:A:169:GLY:HA3	2.17	0.44
1:A:240:HIS:NE2	1:A:244:GLU:OE2	2.51	0.44
1:C:161:TYR:O	1:C:170:PHE:N	2.51	0.44
1:G:266:ARG:NH2	1:G:437:ASP:O	2.51	0.44
1:A:215:PHE:CE2	1:A:225:ASN:HB2	2.53	0.43
1:A:265:GLU:O	1:A:268:ARG:N	2.50	0.43
1:G:197:ARG:O	1:G:214:PHE:N	2.50	0.43
1:G:200:VAL:CG2	1:G:211:GLY:HA3	2.49	0.43
1:G:141:ILE:HD11	1:G:148:VAL:CG2	2.48	0.43
1:G:270:ILE:HG22	1:G:274:ARG:HD2	2.01	0.43
1:G:35:LEU:HB3	1:G:42:TYR:CE2	2.53	0.43
1:A:308:LEU:HB3	1:A:315:PRO:HG3	2.00	0.43
1:C:174:LEU:HD11	1:C:216:VAL:HG21	2.00	0.43
1:A:30:GLU:HA	1:A:33:ARG:NH1	2.34	0.43
1:G:179:ILE:O	1:G:183:GLY:N	2.51	0.43
1:E:305:PHE:CZ	1:E:315:PRO:HB2	2.53	0.43
1:G:245:PHE:HD2	1:G:246:MET:HE2	1.84	0.43
1:A:91:GLU:OE1	1:A:93:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ILE:O	1:C:169:GLY:HA3	2.18	0.43
1:E:3:VAL:HG22	1:E:249:PRO:HG2	2.00	0.43
1:G:265:GLU:O	1:G:268:ARG:N	2.50	0.43
2:D:4:C:H1'	2:D:32:G:N2	2.34	0.42
2:B:22:U:H2'	2:B:23:G:C8	2.54	0.42
1:E:274:ARG:NH2	1:E:433:MET:O	2.49	0.42
2:B:12:G:H2'	2:B:13:U:O4'	2.19	0.42
1:C:217:VAL:CG2	1:C:222:GLU:HA	2.48	0.42
1:G:278:VAL:HG22	1:G:332:GLU:HG3	2.01	0.42
1:G:344:ARG:CZ	2:H:14:U:H5"	2.49	0.42
1:C:411:TYR:O	1:C:412:PHE:HB3	2.19	0.42
1:C:13:LEU:O	1:C:55:LYS:HD3	2.19	0.42
1:A:321:LYS:HD3	1:A:322:ALA:N	2.35	0.41
1:A:368:PHE:O	1:A:375:TRP:N	2.50	0.41
1:A:218:ASP:HB3	1:A:221:ASP:O	2.21	0.41
1:E:261:GLU:OE1	1:E:426:THR:HG23	2.20	0.41
1:G:161:TYR:O	1:G:170:PHE:O	2.38	0.41
1:G:361:ARG:HD3	1:G:363:ARG:CZ	2.51	0.41
1:G:25:ARG:O	1:G:29:GLU:N	2.47	0.41
1:G:299:ARG:O	1:G:303:LYS:HG2	2.20	0.41
1:E:200:VAL:CG2	1:E:211:GLY:HA3	2.50	0.41
1:G:160:ILE:O	1:G:169:GLY:HA3	2.20	0.41
2:D:10:A:C2	2:D:23:G:C2	3.09	0.41
1:G:165:TYR:HE1	1:G:168:ARG:NH2	2.18	0.41
2:B:17:A:H4'	2:B:18:G:OP1	2.21	0.41
1:C:170:PHE:N	1:C:170:PHE:CD1	2.89	0.41
1:C:361:ARG:NH2	2:D:14:U:OP1	2.54	0.41
2:D:11:G:N3	2:D:11:G:H2'	2.37	0.41
1:E:199:THR:O	1:E:214:PHE:HA	2.21	0.41
2:B:16:G:N1	2:B:17:A:C2	2.89	0.40
1:C:263:GLU:HG2	1:C:266:ARG:H	1.86	0.40
1:A:411:TYR:CG	1:A:412:PHE:N	2.88	0.40
2:B:29:A:C3'	2:B:30:U:H5'	2.47	0.40
2:D:24:C:H2'	2:D:25:C:H6	1.86	0.40
1:A:170:PHE:CD1	1:A:170:PHE:N	2.90	0.40
1:C:83:GLY:HA3	1:C:100:VAL:HG21	2.04	0.40
1:E:171:SER:O	1:E:174:LEU:HB3	2.21	0.40
1:A:349:PHE:CD2	1:C:236:ALA:HA	2.56	0.40
1:C:38:LEU:HB2	1:C:40:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/457 (95%)	420 (97%)	15 (3%)	0	100	100
1	C	430/457 (94%)	415 (96%)	15 (4%)	0	100	100
1	E	424/457 (93%)	406 (96%)	18 (4%)	0	100	100
1	G	424/457 (93%)	407 (96%)	17 (4%)	0	100	100
All	All	1713/1828 (94%)	1648 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/404 (96%)	383 (99%)	4 (1%)	76	91
1	C	384/404 (95%)	382 (100%)	2 (0%)	88	96
1	E	379/404 (94%)	378 (100%)	1 (0%)	92	97
1	G	378/404 (94%)	376 (100%)	2 (0%)	88	96
All	All	1528/1616 (95%)	1519 (99%)	9 (1%)	86	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	PHE
1	A	222	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	223	LYS
1	A	350	GLU
1	C	53	TRP
1	C	224	ARG
1	E	72	LYS
1	G	170	PHE
1	G	301	SER

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

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	35/36 (97%)	9 (25%)	4 (11%)
2	D	27/36 (75%)	2 (7%)	0
2	F	25/36 (69%)	3 (12%)	0
2	H	25/36 (69%)	1 (4%)	0
All	All	112/144 (77%)	15 (13%)	4 (3%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	17	A
2	B	18	G
2	B	19	U
2	B	28	G
2	B	29	A
2	B	30	U
2	B	31	C
2	B	32	G
2	B	36	C
2	D	11	G
2	D	26	G
2	F	17	A
2	F	18	G
2	F	19	U
2	H	8	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	17	A
2	B	18	G
2	B	28	G
2	B	29	A

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)

10 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	$\#\|Z\| > 2$
3	SO4	E	502	-	4,4,4	0.14	0	6,6,6	0.19	0
3	SO4	A	502	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	G	501	-	4,4,4	0.19	0	6,6,6	0.20	0
3	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.37	0
3	SO4	G	502	-	4,4,4	0.21	0	6,6,6	0.15	0
3	SO4	A	501	-	4,4,4	0.22	0	6,6,6	0.21	0
3	SO4	E	501	-	4,4,4	0.19	0	6,6,6	0.08	0
3	SO4	A	503	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SO4	A	504	-	4,4,4	0.16	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	SO4	1	0
3	A	505	SO4	1	0
3	A	504	SO4	1	0

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	437/457 (95%)	-0.20	3 (0%) 87 69	26, 49, 108, 138	0
1	C	434/457 (94%)	-0.20	4 (0%) 84 63	27, 49, 109, 141	0
1	E	428/457 (93%)	-0.21	3 (0%) 87 69	28, 50, 108, 144	0
1	G	428/457 (93%)	-0.19	5 (1%) 79 54	29, 50, 109, 184	0
2	B	36/36 (100%)	0.22	2 (5%) 24 8	51, 106, 171, 201	0
2	D	30/36 (83%)	-0.02	0 100 100	48, 96, 139, 162	0
2	F	27/36 (75%)	0.08	0 100 100	49, 97, 140, 161	0
2	H	28/36 (77%)	-0.03	0 100 100	63, 107, 131, 137	0
All	All	1848/1972 (93%)	-0.18	17 (0%) 84 63	26, 51, 114, 201	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	122	ASN	5.6
1	C	125	SER	4.4
1	G	95	ALA	3.3
1	C	73	GLU	3.2
1	G	90	TYR	3.0
2	B	30	U	2.8
1	A	73	GLU	2.7
1	G	73	GLU	2.5
1	C	123	ILE	2.4
1	A	258	HIS	2.4
1	E	114	CYS	2.3
1	G	114	CYS	2.3
1	G	84	LYS	2.3
1	A	5	GLU	2.2
1	C	65	LEU	2.1
2	B	29	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	71	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 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. 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	SO4	G	501	5/5	0.94	0.18	47,60,65,65	0
3	SO4	A	505	5/5	0.96	0.15	73,73,75,77	0
3	SO4	A	503	5/5	0.96	0.15	55,62,65,67	0
3	SO4	C	501	5/5	0.97	0.16	34,43,49,60	0
3	SO4	G	502	5/5	0.97	0.12	57,61,66,66	0
3	SO4	A	502	5/5	0.97	0.09	57,61,65,68	0
3	SO4	A	501	5/5	0.98	0.18	48,52,55,57	0
3	SO4	E	501	5/5	0.98	0.14	52,61,62,62	0
3	SO4	E	502	5/5	0.98	0.11	59,61,66,68	0
3	SO4	A	504	5/5	0.98	0.12	60,64,72,77	0

6.5 Other polymers (i)

There are no such residues in this entry.