Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 12:30 PM JST

PDB ID	:	5HC9
Title	:	Thermotoga maritima CCA-adding enzyme complexed with tRNA_CCA
Authors	:	Yamashita, S.; Tomita, K.
Deposited on	:	2016-01-04
Resolution	:	2.90 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:

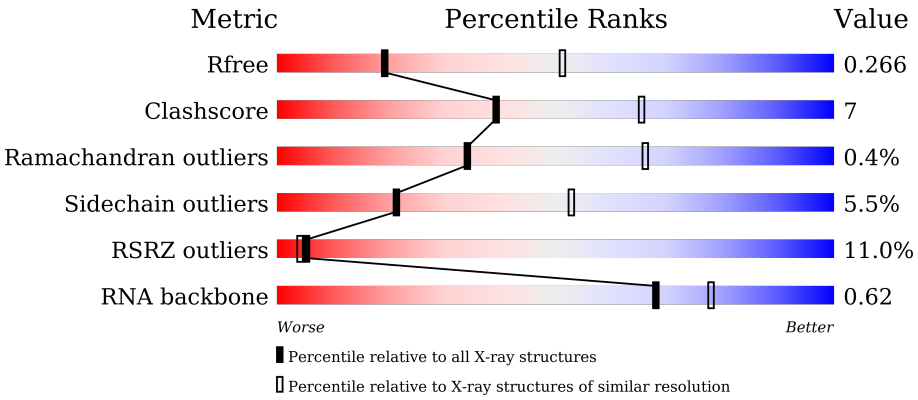
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	441	5% 73% 20%
1	B	441	5% 72% 18% 7%
2	C	76	49% 57% 37% 7%
2	D	76	32% 58% 33% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10128 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 tRNA nucleotidyl transferase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3502	2264	591	636	11			
1	B	410	Total	C	N	O	S	0	0	0
			3378	2183	575	610	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9WZH4
A	429	LYS	-	expression tag	UNP Q9WZH4
A	430	LEU	-	expression tag	UNP Q9WZH4
A	431	ALA	-	expression tag	UNP Q9WZH4
A	432	ALA	-	expression tag	UNP Q9WZH4
A	433	ALA	-	expression tag	UNP Q9WZH4
A	434	LEU	-	expression tag	UNP Q9WZH4
A	435	GLU	-	expression tag	UNP Q9WZH4
A	436	HIS	-	expression tag	UNP Q9WZH4
A	437	HIS	-	expression tag	UNP Q9WZH4
A	438	HIS	-	expression tag	UNP Q9WZH4
A	439	HIS	-	expression tag	UNP Q9WZH4
A	440	HIS	-	expression tag	UNP Q9WZH4
A	441	HIS	-	expression tag	UNP Q9WZH4
B	1	MET	-	initiating methionine	UNP Q9WZH4
B	429	LYS	-	expression tag	UNP Q9WZH4
B	430	LEU	-	expression tag	UNP Q9WZH4
B	431	ALA	-	expression tag	UNP Q9WZH4
B	432	ALA	-	expression tag	UNP Q9WZH4
B	433	ALA	-	expression tag	UNP Q9WZH4
B	434	LEU	-	expression tag	UNP Q9WZH4
B	435	GLU	-	expression tag	UNP Q9WZH4
B	436	HIS	-	expression tag	UNP Q9WZH4
B	437	HIS	-	expression tag	UNP Q9WZH4
B	438	HIS	-	expression tag	UNP Q9WZH4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	439	HIS	-	expression tag	UNP Q9WZH4
B	440	HIS	-	expression tag	UNP Q9WZH4
B	441	HIS	-	expression tag	UNP Q9WZH4

- Molecule 2 is a RNA chain called tRNAphe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	76	Total	C	N	O	P	0	0	0
			1623	723	291	533	76			
2	D	76	Total	C	N	O	P	0	0	0
			1623	723	291	533	76			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

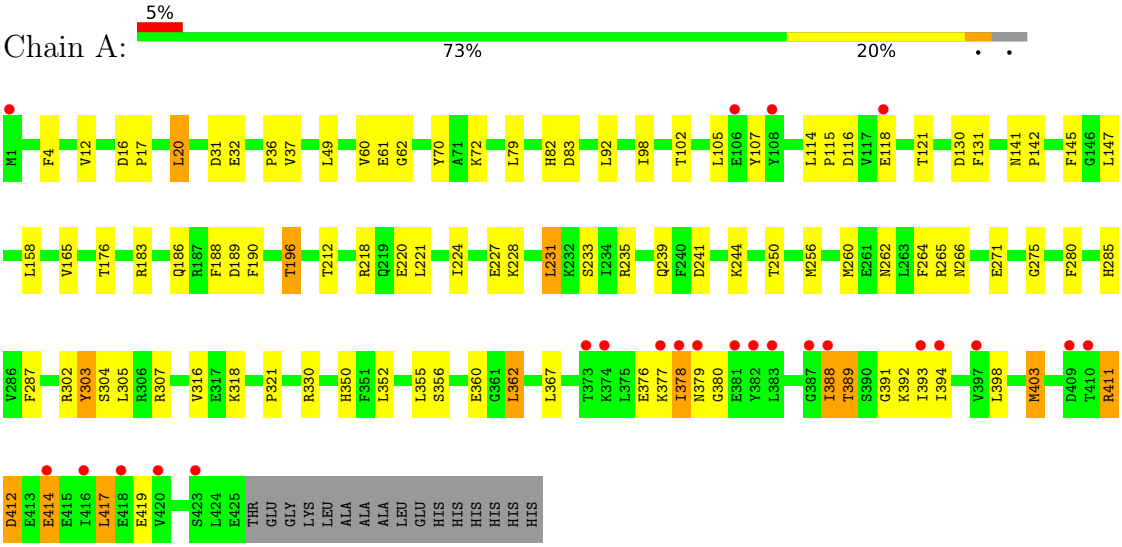
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

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.

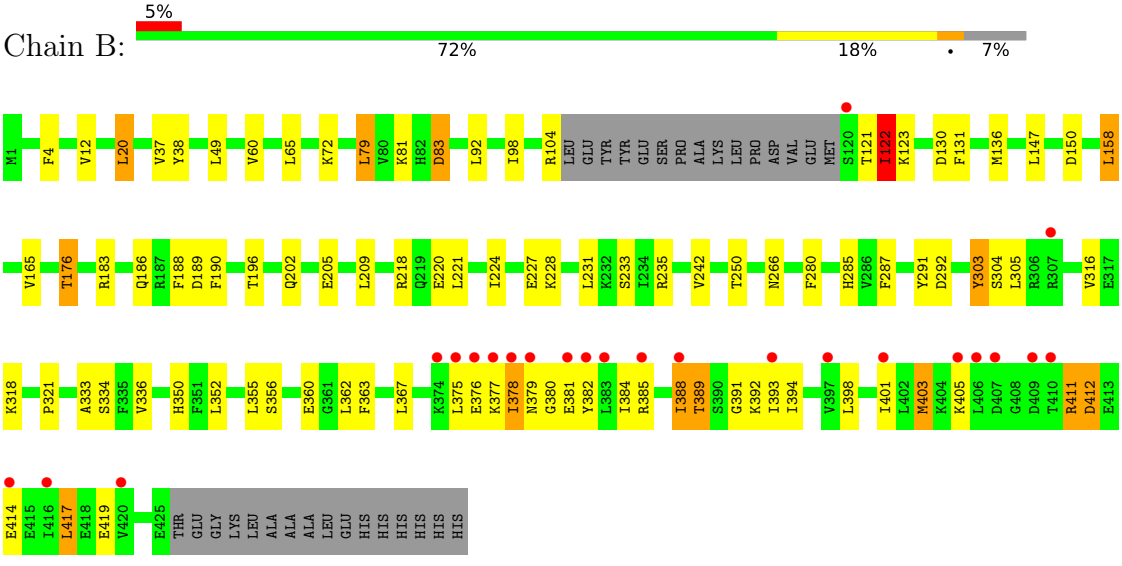
• Molecule 1: tRNA nucleotidyl transferase-related protein

Chain A:



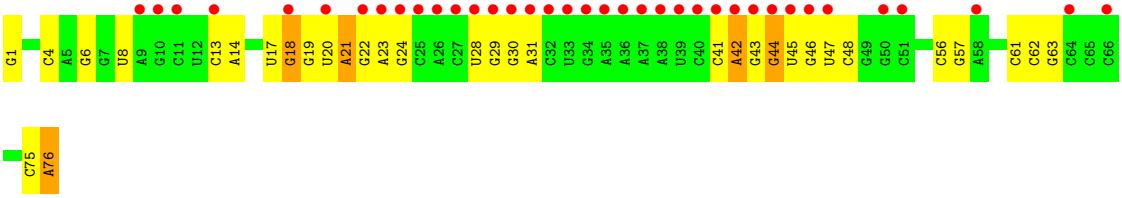
• Molecule 1: tRNA nucleotidyl transferase-related protein

Chain B:

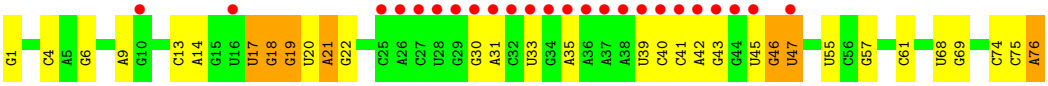


• Molecule 2: tRNAphe

Chain C:



• Molecule 2: tRNAphe



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.18Å 96.19Å 108.58Å 90.00° 110.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 48.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.90) 99.7 (48.78-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.264 0.221 , 0.266	Depositor DCC
R_{free} test set	2112 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 74.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10128	wwPDB-VP
Average B, all atoms (Å^2)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: MG

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	0.23	0/3568	0.42	0/4798
1	B	0.23	0/3439	0.42	0/4620
2	C	0.28	1/1813 (0.1%)	0.67	0/2823
2	D	0.28	1/1813 (0.1%)	0.67	0/2823
All	All	0.25	2/10633 (0.0%)	0.53	0/15064

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	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	G	OP3-P	-10.57	1.48	1.61
2	D	1	G	OP3-P	-10.43	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	ASP	Peptide
1	B	412	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	B	83	ASP	Peptide

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	3502	0	3596	58	0
1	B	3378	0	3478	53	0
2	C	1623	0	822	18	0
2	D	1623	0	822	19	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	10128	0	8718	140	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 7.

All (140) 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:218:ARG:NH2	1:A:304:SER:O	2.24	0.71
1:A:411:ARG:NH2	1:A:419:GLU:OE2	2.26	0.69
1:B:12:VAL:HA	1:B:20:LEU:HD11	1.74	0.68
1:A:379:ASN:ND2	2:C:56:C:OP1	2.27	0.67
1:A:32:GLU:OE2	1:A:70:TYR:OH	2.10	0.66
1:A:379:ASN:HA	1:A:398:LEU:HD21	1.77	0.66
2:C:76:A:OP1	2:C:76:A:H8	1.78	0.65
1:A:218:ARG:NH2	2:C:4:C:O2'	2.30	0.64
1:B:218:ARG:NH2	1:B:304:SER:O	2.32	0.63
2:D:14:A:H61	2:D:21:A:H2	1.45	0.62
1:A:318:LYS:HG3	1:B:321:PRO:HB2	1.81	0.62
2:C:18:G:HO2'	2:C:57:G:H22	1.45	0.61
1:A:321:PRO:HB2	1:B:318:LYS:HG3	1.82	0.61
1:A:262:ASN:OD1	1:A:265:ARG:NH1	2.33	0.61
1:A:307:ARG:NH2	2:C:14:A:OP1	2.32	0.60
2:C:18:G:HO2'	2:C:57:G:N2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HA	1:A:20:LEU:HD11	1.85	0.58
2:D:75:C:H3'	2:D:76:A:H5"	1.86	0.58
2:D:18:G:O2'	2:D:57:G:N2	2.28	0.57
2:D:46:G:H4'	2:D:47:U:OP2	2.03	0.57
1:A:165:VAL:HG22	1:A:196:THR:HB	1.87	0.56
1:B:218:ARG:NH2	2:D:4:C:O2'	2.39	0.56
1:A:49:LEU:HD21	1:A:158:LEU:HD22	1.88	0.56
1:A:266:ASN:HB3	1:A:352:LEU:HD13	1.87	0.55
1:B:165:VAL:HG22	1:B:196:THR:HB	1.88	0.55
1:A:4:PHE:HB3	1:A:147:LEU:HD11	1.89	0.55
1:A:105:LEU:HG	1:A:121:THR:HG22	1.88	0.55
2:C:75:C:H3'	2:C:76:A:H5"	1.87	0.54
1:B:392:LYS:HG2	2:D:19:G:C4	2.42	0.54
2:D:18:G:H1	2:D:55:U:H1'	1.72	0.54
1:A:176:THR:HG22	1:A:220:GLU:HG3	1.88	0.54
1:B:266:ASN:HB3	1:B:352:LEU:HD13	1.90	0.53
2:D:42:A:H2'	2:D:43:G:H8	1.73	0.53
1:B:334:SER:HB2	1:B:403:MET:HG3	1.90	0.53
1:A:31:ASP:OD2	1:A:142:PRO:HD2	2.09	0.52
1:B:209:LEU:HD21	1:B:242:VAL:HG13	1.90	0.52
1:B:411:ARG:NH2	1:B:419:GLU:OE2	2.43	0.52
1:B:176:THR:HG22	1:B:220:GLU:HG3	1.90	0.51
2:C:30:G:H2'	2:C:31:A:H8	1.75	0.51
1:A:241:ASP:HB3	1:A:244:LYS:HE2	1.91	0.51
2:C:18:G:O2'	2:C:57:G:N2	2.31	0.51
1:A:37:VAL:HG22	1:A:60:VAL:HG12	1.92	0.51
1:B:376:GLU:N	1:B:376:GLU:OE2	2.44	0.51
1:A:212:THR:O	1:A:302:ARG:NH1	2.43	0.51
1:B:136:MET:HG2	1:B:150:ASP:HB2	1.93	0.49
1:B:130:ASP:N	2:D:76:A:OP2	2.45	0.49
1:A:376:GLU:HG2	1:A:377:LYS:H	1.77	0.49
1:B:375:LEU:HA	1:B:405:LYS:NZ	2.28	0.49
1:A:186:GLN:HG3	1:A:233:SER:OG	2.13	0.48
1:A:352:LEU:HD23	1:A:355:LEU:HD11	1.95	0.48
1:B:186:GLN:HG3	1:B:233:SER:OG	2.14	0.48
1:A:393:ILE:H	1:A:393:ILE:HD12	1.78	0.48
1:B:356:SER:HA	1:B:360:GLU:HB2	1.95	0.48
1:B:37:VAL:HG22	1:B:60:VAL:HG12	1.96	0.48
2:D:42:A:H2'	2:D:43:G:C8	2.48	0.48
1:B:393:ILE:H	1:B:393:ILE:HD12	1.79	0.48
1:B:227:GLU:HG3	1:B:228:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLY:O	1:B:394:ILE:HG12	2.13	0.47
1:B:65:LEU:HD22	1:B:81:LYS:HB3	1.95	0.47
1:A:141:ASN:O	1:A:145:PHE:N	2.48	0.47
1:B:38:TYR:CE1	1:B:122:ILE:HG13	2.49	0.47
1:B:250:THR:HG22	1:B:287:PHE:O	2.15	0.47
1:B:414:GLU:HA	1:B:417:LEU:HB2	1.95	0.47
1:B:72:LYS:HD2	1:B:79:LEU:HB2	1.97	0.47
1:B:316:VAL:HG11	1:B:350:HIS:CG	2.49	0.47
1:B:379:ASN:HA	1:B:398:LEU:HD11	1.97	0.47
1:A:392:LYS:HB2	1:A:392:LYS:NZ	2.29	0.46
1:B:4:PHE:HB3	1:B:147:LEU:HD11	1.98	0.46
1:B:189:ASP:O	1:B:190:PHE:HD2	1.99	0.46
2:C:8:U:H4'	2:C:48:C:H4'	1.98	0.46
1:A:36:PRO:HD2	1:A:61:GLU:HB2	1.99	0.45
2:D:30:G:H2'	2:D:31:A:C8	2.51	0.45
1:A:391:GLY:O	1:A:394:ILE:HG12	2.16	0.45
1:A:403:MET:HE3	1:A:403:MET:HA	1.97	0.45
1:B:388:ILE:HG22	1:B:389:THR:H	1.82	0.45
2:C:44:G:OP2	2:C:44:G:H8	2.00	0.45
2:D:17:U:O5'	2:D:18:G:H5'	2.16	0.45
1:A:388:ILE:HG22	1:A:389:THR:H	1.81	0.45
1:A:355:LEU:HD13	1:A:360:GLU:HA	1.98	0.44
1:A:130:ASP:OD2	1:A:131:PHE:N	2.42	0.44
1:B:292:ASP:OD1	1:B:292:ASP:N	2.46	0.44
1:A:16:ASP:OD2	1:A:17:PRO:HD2	2.17	0.44
1:B:49:LEU:HD21	1:B:158:LEU:HD22	2.00	0.44
1:A:227:GLU:HG3	1:A:228:LYS:H	1.82	0.44
1:A:189:ASP:O	1:A:190:PHE:HD2	2.01	0.43
1:A:218:ARG:HG3	1:A:280:PHE:CZ	2.53	0.43
1:A:158:LEU:HD23	1:A:158:LEU:HA	1.84	0.43
2:C:23:A:H2'	2:C:24:G:C8	2.54	0.43
2:C:14:A:H61	2:C:21:A:H2	1.66	0.43
1:A:376:GLU:HG2	1:A:377:LYS:N	2.34	0.43
1:B:231:LEU:HD11	1:B:235:ARG:CZ	2.47	0.43
1:A:377:LYS:HA	1:A:377:LYS:HD3	1.69	0.43
1:A:183:ARG:HB2	1:A:224:ILE:HG12	1.99	0.43
1:A:141:ASN:HA	1:A:142:PRO:HD3	1.90	0.43
1:B:376:GLU:HG2	1:B:377:LYS:N	2.34	0.43
1:B:379:ASN:OD1	1:B:380:GLY:N	2.51	0.43
2:D:41:C:H2'	2:D:42:A:C8	2.53	0.43
2:D:76:A:OP1	2:D:76:A:H8	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLY:O	1:A:102:THR:HG23	2.19	0.43
1:A:250:THR:HG22	1:A:287:PHE:O	2.19	0.42
1:B:303:TYR:O	1:B:305:LEU:HG	2.18	0.42
1:B:376:GLU:OE2	1:B:405:LYS:NZ	2.49	0.42
2:D:68:U:H2'	2:D:69:G:C8	2.55	0.42
1:A:231:LEU:HG	1:A:264:PHE:HD1	1.83	0.42
1:B:130:ASP:OD2	1:B:131:PHE:N	2.50	0.42
1:B:376:GLU:HG2	1:B:377:LYS:H	1.84	0.42
1:B:378:ILE:HG23	1:B:382:TYR:HD2	1.83	0.42
2:D:68:U:H2'	2:D:69:G:H8	1.84	0.42
2:C:30:G:H2'	2:C:31:A:C8	2.52	0.42
2:D:33:U:H2'	2:D:35:A:OP2	2.20	0.42
1:A:303:TYR:O	1:A:305:LEU:HG	2.19	0.42
1:A:330:ARG:HD2	1:A:362:LEU:HD11	2.02	0.42
1:B:398:LEU:O	1:B:401:ILE:HG12	2.20	0.42
1:B:202:GLN:HA	1:B:205:GLU:HG2	2.02	0.42
1:B:381:GLU:O	1:B:385:ARG:HG2	2.20	0.42
1:A:92:LEU:HD11	1:A:98:ILE:HD11	2.02	0.41
1:A:271:GLU:HA	1:A:275:GLY:O	2.20	0.41
1:A:414:GLU:HA	1:A:417:LEU:HB2	2.02	0.41
1:A:114:LEU:HB3	1:A:115:PRO:HD2	2.02	0.41
1:A:378:ILE:HD13	1:A:417:LEU:HD12	2.03	0.41
1:A:379:ASN:HD22	1:A:380:GLY:H	1.68	0.41
1:B:183:ARG:HB2	1:B:224:ILE:HG12	2.02	0.41
2:C:62:C:H2'	2:C:63:G:H8	1.85	0.41
1:A:256:MET:O	1:A:260:MET:HG2	2.21	0.41
1:A:316:VAL:HG11	1:A:350:HIS:CG	2.56	0.41
1:B:363:PHE:O	1:B:367:LEU:HB2	2.21	0.41
1:B:379:ASN:HA	1:B:398:LEU:HD21	2.03	0.41
1:B:380:GLY:O	1:B:384:ILE:HG13	2.21	0.41
1:B:121:THR:C	1:B:123:LYS:H	2.24	0.41
2:C:62:C:H2'	2:C:63:G:C8	2.56	0.41
2:D:39:U:H2'	2:D:40:C:C6	2.56	0.41
1:B:333:ALA:HA	1:B:336:VAL:HG22	2.02	0.40
1:A:356:SER:HA	1:A:360:GLU:HB2	2.03	0.40
2:C:41:C:H2'	2:C:42:A:O4'	2.21	0.40
1:A:105:LEU:C	1:A:107:TYR:H	2.24	0.40
1:B:221:LEU:HD23	1:B:280:PHE:HE1	1.87	0.40
2:C:28:U:H2'	2:C:29:G:C8	2.57	0.40
2:D:30:G:H2'	2:D:31:A:H8	1.86	0.40
1:A:235:ARG:O	1:A:239:GLN:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD11	1:B:98:ILE:HD11	2.03	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	423/441 (96%)	398 (94%)	24 (6%)	1 (0%)	47 78
1	B	406/441 (92%)	382 (94%)	22 (5%)	2 (0%)	29 61
All	All	829/882 (94%)	780 (94%)	46 (6%)	3 (0%)	34 66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	ILE
1	A	378	ILE
1	B	378	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	383/395 (97%)	361 (94%)	22 (6%)	20 51
1	B	369/395 (93%)	350 (95%)	19 (5%)	24 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	752/790 (95%)	711 (94%)	41 (6%)	21 53

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	72	LYS
1	A	79	LEU
1	A	82	HIS
1	A	83	ASP
1	A	116	ASP
1	A	118	GLU
1	A	188	PHE
1	A	196	THR
1	A	221	LEU
1	A	231	LEU
1	A	285	HIS
1	A	303	TYR
1	A	362	LEU
1	A	367	LEU
1	A	388	ILE
1	A	389	THR
1	A	403	MET
1	A	411	ARG
1	A	412	ASP
1	A	414	GLU
1	A	417	LEU
1	B	20	LEU
1	B	79	LEU
1	B	83	ASP
1	B	104	ARG
1	B	122	ILE
1	B	158	LEU
1	B	176	THR
1	B	188	PHE
1	B	285	HIS
1	B	291	TYR
1	B	303	TYR
1	B	355	LEU
1	B	362	LEU
1	B	388	ILE
1	B	389	THR

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Mol	Chain	Res	Type
1	B	403	MET
1	B	411	ARG
1	B	412	ASP
1	B	417	LEU

Sometimes 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	C	75/76 (98%)	15 (20%)	3 (4%)
2	D	75/76 (98%)	14 (18%)	4 (5%)
All	All	150/152 (98%)	29 (19%)	7 (4%)

All (29) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	G
2	C	13	C
2	C	17	U
2	C	18	G
2	C	19	G
2	C	20	U
2	C	22	G
2	C	42	A
2	C	43	G
2	C	44	G
2	C	45	U
2	C	46	G
2	C	47	U
2	C	61	C
2	C	76	A
2	D	6	G
2	D	9	A
2	D	13	C
2	D	17	U
2	D	18	G
2	D	19	G
2	D	20	U
2	D	22	G

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Mol	Chain	Res	Type
2	D	45	U
2	D	46	G
2	D	47	U
2	D	61	C
2	D	74	C
2	D	76	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	19	G
2	C	21	A
2	C	46	G
2	D	19	G
2	D	21	A
2	D	45	U
2	D	46	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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^{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	425/441 (96%)	0.56	24 (5%)	24	20	48, 82, 210, 261	0
1	B	410/441 (92%)	0.52	24 (5%)	22	18	48, 79, 188, 278	0
2	C	76/76 (100%)	2.51	37 (48%)	0	0	99, 221, 341, 369	0
2	D	76/76 (100%)	1.53	24 (31%)	0	0	61, 185, 327, 342	0
All	All	987/1034 (95%)	0.77	109 (11%)	5	4	48, 88, 248, 369	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	34	G	11.0
1	B	388	ILE	9.3
2	C	35	A	9.0
2	C	37	A	7.9
2	C	40	C	7.7
1	A	387	GLY	7.5
2	C	31	A	7.0
2	D	32	C	6.9
2	C	32	C	6.8
2	D	34	G	6.4
2	D	31	A	6.4
2	C	47	U	6.2
2	C	20	U	5.2
2	D	30	G	5.2
1	B	379	ASN	5.1
2	D	28	U	5.0
2	C	45	U	5.0
2	C	38	A	4.9
2	C	36	A	4.9
2	C	30	G	4.8
2	D	33	U	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	41	C	4.7
2	C	41	C	4.6
2	D	36	A	4.6
1	A	374	LYS	4.6
2	C	33	U	4.5
1	B	420	VAL	4.3
2	D	43	G	4.3
1	A	410	THR	4.2
2	C	44	G	4.2
2	D	45	U	4.2
1	A	416	ILE	4.1
1	B	385	ARG	4.1
1	B	377	LYS	4.1
2	C	39	U	4.0
1	A	423	SER	4.0
2	D	37	A	3.9
2	D	42	A	3.9
1	A	383	LEU	3.9
1	A	418	GLU	3.9
1	A	420	VAL	3.8
1	B	374	LYS	3.8
2	D	29	G	3.8
2	D	26	A	3.8
1	A	388	ILE	3.7
2	C	29	G	3.7
2	C	43	G	3.5
1	B	397	VAL	3.5
1	B	381	GLU	3.5
1	A	394	ILE	3.4
2	D	27	C	3.4
2	C	25	C	3.4
2	C	23	A	3.3
2	D	40	C	3.3
2	C	28	U	3.2
1	A	414	GLU	3.2
2	C	10	G	3.2
1	B	401	ILE	3.2
1	B	410	THR	3.2
2	D	44	G	3.1
2	C	26	A	3.1
1	A	118	GLU	3.1
2	D	25	C	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	378	ILE	3.0
1	B	407	ASP	3.0
1	A	379	ASN	3.0
1	A	381	GLU	2.9
1	B	406	LEU	2.8
2	C	50	G	2.8
1	B	393	ILE	2.8
2	C	66	C	2.8
2	D	47	U	2.8
1	B	409	ASP	2.7
2	C	42	A	2.7
1	A	377	LYS	2.7
2	C	46	G	2.7
2	D	38	A	2.7
1	A	106	GLU	2.6
1	A	393	ILE	2.6
2	D	35	A	2.5
2	D	16	U	2.5
2	C	58	A	2.5
1	B	120	SER	2.4
2	C	51	C	2.4
1	A	409	ASP	2.4
1	B	416	ILE	2.4
2	C	22	G	2.3
2	C	24	G	2.3
2	D	39	U	2.3
2	C	13	C	2.3
1	A	397	VAL	2.2
1	B	376	GLU	2.2
2	C	27	C	2.2
2	C	11	C	2.2
1	B	375	LEU	2.2
2	C	64	C	2.2
1	B	414	GLU	2.2
1	A	108	TYR	2.1
1	A	382	TYR	2.1
1	B	383	LEU	2.1
1	A	1	MET	2.1
2	C	9	A	2.1
2	C	18	G	2.1
1	A	373	THR	2.1
2	D	10	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	307	ARG	2.0
1	A	378	ILE	2.0
1	B	382	TYR	2.0
1	B	405	LYS	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	MG	A	1001	1/1	0.86	0.36	62,62,62,62	0
3	MG	B	1001	1/1	0.95	0.42	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.