



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:47 AM GMT

PDB ID : 3Q0J  
Title : Crystal Structure of the Mycobacterium tuberculosis Crotonase in complex with the Inhibitor AcetoacetylCoA  
Authors : Bruning, J.B.; Delgado, E.; Ghosh, S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2010-12-15  
Resolution : 2.40 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

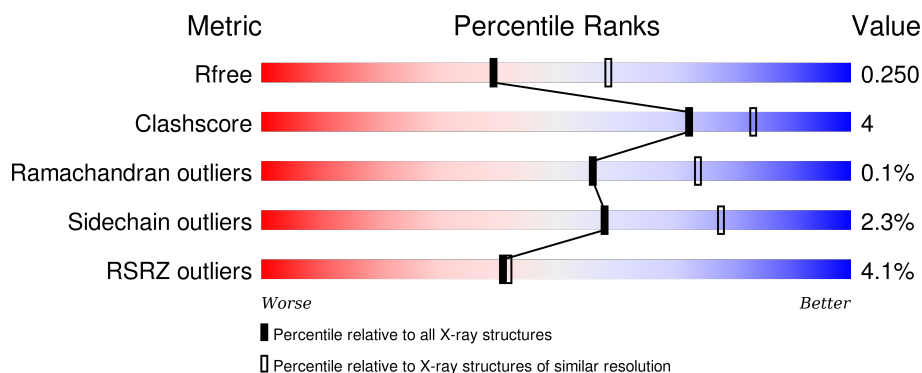
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	258	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>
1	B	258	<div> <div>5%</div> <div>93%</div> <div>5%</div> </div>
1	C	258	<div> <div>4%</div> <div>88%</div> <div>11%</div> </div>
1	D	258	<div> <div>5%</div> <div>86%</div> <div>13%</div> </div>
1	E	258	<div> <div>5%</div> <div>89%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	258	<div><div></div><div>2%</div><div>91%</div><div>7% ..</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12306 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.

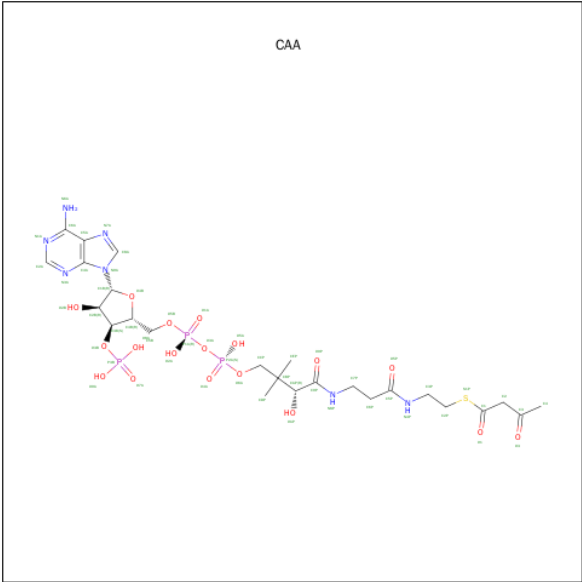
- Molecule 1 is a protein called enoyl-CoA hydratase echA8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	2	0
			1872	1166	324	370	12			
1	B	255	Total	C	N	O	S	0	2	0
			1885	1175	324	374	12			
1	C	255	Total	C	N	O	S	0	0	0
			1875	1170	325	368	12			
1	D	255	Total	C	N	O	S	0	1	0
			1879	1172	326	369	12			
1	E	253	Total	C	N	O	S	0	0	0
			1852	1157	321	362	12			
1	F	254	Total	C	N	O	S	0	0	0
			1859	1160	321	366	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P64016
B	0	SER	-	EXPRESSION TAG	UNP P64016
C	0	SER	-	EXPRESSION TAG	UNP P64016
D	0	SER	-	EXPRESSION TAG	UNP P64016
E	0	SER	-	EXPRESSION TAG	UNP P64016
F	0	SER	-	EXPRESSION TAG	UNP P64016

- Molecule 2 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: C<sub>25</sub>H<sub>40</sub>N<sub>7</sub>O<sub>18</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 3 is water.

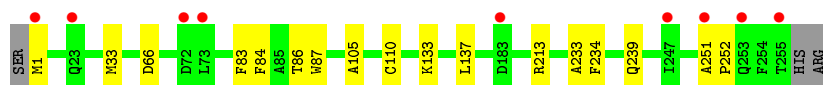
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	171	Total	O	0	0
			171	171		
3	B	173	Total	O	0	0
			173	173		
3	C	178	Total	O	0	0
			178	178		
3	D	141	Total	O	0	0
			141	141		
3	E	133	Total	O	0	0
			133	133		
3	F	180	Total	O	0	0
			180	180		

### 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: enoyl-CoA hydratase echA8

Chain A: 




- Molecule 1: enoyl-CoA hydratase echA8

Chain B: 




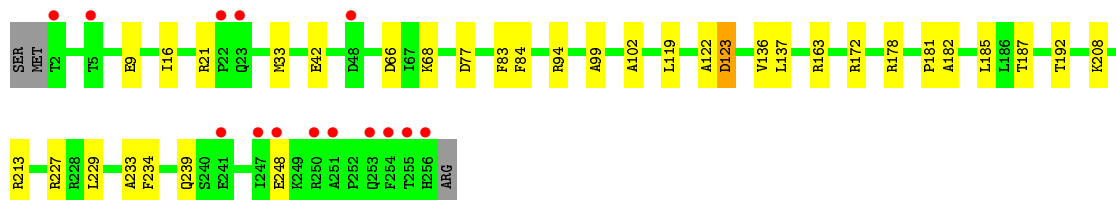
- Molecule 1: enoyl-CoA hydratase echA8

Chain C: 




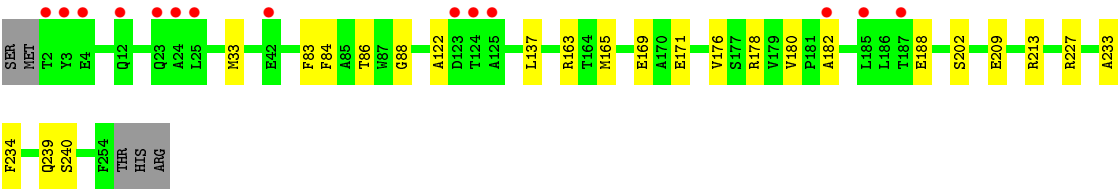
- Molecule 1: enoyl-CoA hydratase echA8

Chain D: 

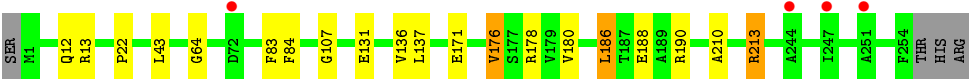
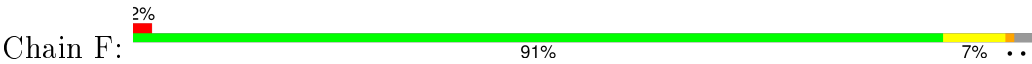


- Molecule 1: enoyl-CoA hydratase echA8

Chain E: 



● Molecule 1: enoyl-CoA hydratase echA8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.96 Å 134.70 Å 134.33 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.42 – 2.40 25.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (26.42-2.40) 98.4 (25.99-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.198 , 0.228 0.226 , 0.250	Depositor DCC
$R_{free}$ test set	3520 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	8 of 69720 reflections (0.011%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.16 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0319e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CAA

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	0.39	0/1901	0.52	0/2571
1	B	0.40	0/1914	0.51	0/2589
1	C	0.40	0/1898	0.53	0/2567
1	D	0.44	1/1906 (0.1%)	0.56	2/2579 (0.1%)
1	E	0.38	0/1875	0.52	0/2538
1	F	0.39	0/1882	0.53	0/2548
All	All	0.40	1/11376 (0.0%)	0.53	2/15392 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	248	GLU	CG-CD	-6.32	1.42	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	248	GLU	CG-CD-OE2	5.55	129.40	118.30
1	D	248	GLU	CA-CB-CG	5.31	125.08	113.40

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	1872	0	1853	13	0
1	B	1885	0	1878	6	0
1	C	1875	0	1873	19	0
1	D	1879	0	1867	19	0
1	E	1852	0	1842	20	0
1	F	1859	0	1845	17	0
2	C	54	0	36	6	0
2	F	54	0	36	9	0
3	A	171	0	0	3	0
3	B	173	0	0	1	0
3	C	178	0	0	4	0
3	D	141	0	0	6	0
3	E	133	0	0	8	0
3	F	180	0	0	0	0
All	All	12306	0	11230	95	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 (95) 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:86:THR:HB	3:E:762:HOH:O	1.45	1.13
1:E:33:MET:SD	3:E:762:HOH:O	2.22	0.96
1:D:33:MET:SD	3:D:562:HOH:O	2.31	0.88
1:C:132:ILE:O	1:C:133:LYS:HG2	1.76	0.85
1:E:180:VAL:HG11	1:E:188:GLU:HG2	1.59	0.84
1:F:84:PHE:CE2	2:F:300:CAA:H4'3	2.14	0.83
1:E:33:MET:HG2	3:E:762:HOH:O	1.83	0.77
1:C:84:PHE:CE2	2:C:300:CAA:H4'3	2.21	0.75
1:B:180:VAL:HG11	1:B:188:GLU:HG2	1.70	0.73
1:F:84:PHE:CZ	2:F:300:CAA:H4'3	2.24	0.72
1:C:126:LYS:HE3	1:C:164:THR:HG21	1.71	0.71
1:E:171:GLU:HB3	3:E:896:HOH:O	1.92	0.70
1:E:33:MET:CE	3:E:762:HOH:O	2.39	0.68
1:B:234:PHE:HA	1:B:239:GLN:HG2	1.76	0.68
1:E:234:PHE:HA	1:E:239:GLN:HG2	1.76	0.66
1:F:131:GLU:CG	2:F:300:CAA:H2'2	2.25	0.66
2:C:300:CAA:P3B	3:C:713:HOH:O	2.54	0.66
1:F:186:LEU:O	1:F:190:ARG:HG2	1.96	0.65
1:D:234:PHE:HA	1:D:239:GLN:HG2	1.79	0.62
1:D:227:ARG:NH2	3:D:745:HOH:O	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:HA	1:A:239:GLN:HG2	1.83	0.60
1:B:83:PHE:O	1:B:84:PHE:HB2	2.01	0.59
1:F:131:GLU:HG3	2:F:300:CAA:H2'2	1.85	0.58
1:C:134:LEU:HD11	2:C:300:CAA:H31	1.85	0.58
1:A:252:PRO:HG3	3:C:796:HOH:O	2.05	0.57
1:D:77:ASP:OD2	3:D:720:HOH:O	2.18	0.57
1:C:132:ILE:O	1:C:133:LYS:CG	2.51	0.56
1:D:99:ALA:HB3	1:D:119[A]:LEU:CD1	2.35	0.56
2:C:300:CAA:O9P	2:C:300:CAA:H61	2.05	0.56
1:A:233:ALA:O	1:A:239:GLN:HG2	2.06	0.56
1:A:33:MET:HE2	1:A:84:PHE:HA	1.89	0.55
1:D:163:ARG:HD3	1:E:178:ARG:HH21	1.72	0.55
1:C:171:GLU:HA	1:C:176:VAL:HG22	1.89	0.54
1:E:163:ARG:HD3	1:F:178:ARG:HH21	1.73	0.54
1:D:83:PHE:O	1:D:84:PHE:HB2	2.07	0.54
1:F:131:GLU:HG2	2:F:300:CAA:H2'2	1.89	0.54
1:E:83:PHE:O	1:E:84:PHE:HB2	2.08	0.53
1:F:64:GLY:HA3	2:F:300:CAA:H21	1.91	0.53
1:F:83:PHE:O	1:F:84:PHE:HB2	2.09	0.53
1:C:66:ASP:HA	2:C:300:CAA:N1A	2.24	0.53
1:F:84:PHE:CZ	2:F:300:CAA:C4	2.93	0.52
1:A:83:PHE:O	1:A:84:PHE:HB2	2.09	0.52
1:B:171:GLU:HA	1:B:176:VAL:HG22	1.91	0.52
1:A:33:MET:CE	1:A:84:PHE:HD1	2.23	0.52
1:A:1:MET:N	3:A:553:HOH:O	2.44	0.51
1:B:178:ARG:NH1	3:B:550:HOH:O	2.44	0.50
1:C:83:PHE:O	1:C:84:PHE:HB2	2.12	0.49
1:C:130:PRO:O	1:C:132:ILE:O	2.30	0.49
1:D:233:ALA:O	1:D:239:GLN:HG2	2.12	0.49
1:E:213:ARG:HG2	1:E:213:ARG:HH11	1.77	0.49
1:D:68:LYS:N	3:D:607:HOH:O	2.39	0.48
1:C:154:LYS:HE3	1:C:169:GLU:OE2	2.14	0.48
1:A:133:LYS:NZ	3:A:759:HOH:O	2.46	0.48
1:E:33:MET:CG	3:E:762:HOH:O	2.36	0.47
1:F:171:GLU:HA	1:F:176:VAL:HG22	1.95	0.47
1:D:136:VAL:HG22	1:D:137:LEU:H	1.79	0.47
1:D:21:ARG:NH2	3:D:941:HOH:O	2.43	0.47
1:A:33:MET:SD	1:A:86:THR:HB	2.55	0.46
1:F:107:GLY:HA2	1:F:131:GLU:OE2	2.15	0.46
1:D:99:ALA:HB3	1:D:119[A]:LEU:HD12	1.96	0.46
1:D:122:ALA:HB1	1:D:182:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ALA:O	1:C:179:VAL:HA	2.16	0.46
1:F:210:ALA:O	1:F:213:ARG:HB2	2.16	0.45
1:C:227:ARG:NH2	3:C:282:HOH:O	2.39	0.45
1:A:33:MET:HE2	1:A:87:TRP:CD1	2.52	0.44
1:E:233:ALA:O	1:E:239:GLN:HG2	2.18	0.44
1:E:171:GLU:HA	1:E:176:VAL:HG22	2.00	0.44
1:D:178:ARG:NH2	1:D:192:THR:OG1	2.51	0.44
1:F:64:GLY:HA3	2:F:300:CAA:H32	2.00	0.43
1:D:94:ARG:O	1:D:208:LYS:HD3	2.18	0.43
1:D:123:ASP:OD2	1:D:181:PRO:HA	2.19	0.43
1:C:89:LYS:HB3	1:C:89:LYS:HE2	1.71	0.43
1:C:46:ASP:HA	1:C:47:PRO:HD3	1.92	0.43
1:E:88:GLY:HA3	3:E:716:HOH:O	2.19	0.42
1:D:102:ALA:HB2	1:D:185:LEU:HD23	2.01	0.42
1:E:209:GLU:O	1:E:213:ARG:HG2	2.20	0.42
2:C:300:CAA:H61	3:C:794:HOH:O	2.18	0.42
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.92	0.42
1:C:103:GLY:H	1:C:124:THR:HG23	1.83	0.42
1:C:150:ILE:HD12	1:C:154:LYS:HB3	2.02	0.41
3:D:732:HOH:O	1:E:227:ARG:NH1	2.54	0.41
1:A:239:GLN:NE2	3:A:893:HOH:O	2.54	0.41
1:C:13:ARG:HA	1:C:48:ASP:O	2.21	0.41
1:A:105:ALA:O	1:A:110:CYS:HB2	2.21	0.41
1:A:251:ALA:HA	1:A:252:PRO:HD3	1.93	0.41
1:F:12:GLN:HB3	1:F:13:ARG:H	1.54	0.41
1:E:122:ALA:HB1	1:E:182:ALA:HA	2.02	0.41
1:C:170:ALA:HB1	1:C:176:VAL:HG13	2.03	0.40
1:E:165:MET:HG3	1:E:169:GLU:HB3	2.03	0.40
1:F:180:VAL:HG11	1:F:188:GLU:HG3	2.02	0.40
1:B:98:ILE:HD11	1:B:196:ILE:HD12	2.02	0.40
1:E:86:THR:CB	3:E:762:HOH:O	2.31	0.40
1:C:132:ILE:O	1:C:133:LYS:CB	2.69	0.40
1:F:64:GLY:HA3	2:F:300:CAA:C3P	2.52	0.40
1:D:9:GLU:HB3	1:D:16:ILE:HG23	2.03	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	255/258 (99%)	250 (98%)	5 (2%)	0	100	100
1	B	255/258 (99%)	248 (97%)	7 (3%)	0	100	100
1	C	253/258 (98%)	247 (98%)	6 (2%)	0	100	100
1	D	254/258 (98%)	245 (96%)	8 (3%)	1 (0%)	39	56
1	E	251/258 (97%)	243 (97%)	8 (3%)	0	100	100
1	F	252/258 (98%)	243 (96%)	8 (3%)	1 (0%)	39	56
All	All	1520/1548 (98%)	1476 (97%)	42 (3%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	123	ASP
1	F	136	VAL

### 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	186/193 (96%)	183 (98%)	3 (2%)	70	86
1	B	189/193 (98%)	184 (97%)	5 (3%)	54	74
1	C	186/193 (96%)	182 (98%)	4 (2%)	60	79
1	D	187/193 (97%)	182 (97%)	5 (3%)	52	73
1	E	182/193 (94%)	179 (98%)	3 (2%)	70	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	183/193 (95%)	177 (97%)	6 (3%)	45 66
All	All	1113/1158 (96%)	1087 (98%)	26 (2%)	58 78

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	137	LEU
1	A	213	ARG
1	B	43	LEU
1	B	178	ARG
1	B	186	LEU
1	B	202	SER
1	B	243	MET
1	C	42	GLU
1	C	137	LEU
1	C	186	LEU
1	C	223	LEU
1	D	42	GLU
1	D	66	ASP
1	D	172	ARG
1	D	187	THR
1	D	213	ARG
1	E	137	LEU
1	E	202	SER
1	E	240	SER
1	F	22	PRO
1	F	43	LEU
1	F	137	LEU
1	F	176	VAL
1	F	186	LEU
1	F	213	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	239	GLN
1	D	34	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	CAA	C	300	-	45,56,56	4.49	18 (40%)	58,83,83	3.26	9 (15%)
2	CAA	F	300	-	45,56,56	4.52	18 (40%)	58,83,83	3.95	9 (15%)

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	CAA	C	300	-	-	0/50/71/71	0/3/3/3
2	CAA	F	300	-	-	0/50/71/71	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	300	CAA	P3B-O9A	-2.07	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	CAA	P1A-O5B	2.03	1.68	1.59
2	C	300	CAA	P3B-O3B	2.16	1.66	1.60
2	F	300	CAA	C6P-C5P	2.50	1.56	1.51
2	C	300	CAA	C5A-N7A	2.77	1.48	1.39
2	F	300	CAA	C5A-N7A	2.85	1.49	1.39
2	F	300	CAA	P3B-O8A	3.08	1.65	1.54
2	C	300	CAA	P3B-O8A	3.13	1.66	1.54
2	C	300	CAA	C1-S1P	3.73	1.84	1.76
2	F	300	CAA	C6A-N6A	3.77	1.46	1.34
2	F	300	CAA	C1-S1P	3.95	1.84	1.76
2	F	300	CAA	P1A-O1A	4.01	1.65	1.51
2	C	300	CAA	C6A-N6A	4.05	1.47	1.34
2	F	300	CAA	P2A-O4A	4.09	1.66	1.51
2	C	300	CAA	P1A-O1A	4.10	1.66	1.51
2	C	300	CAA	P2A-O4A	4.31	1.66	1.51
2	F	300	CAA	P3B-O7A	4.48	1.65	1.51
2	F	300	CAA	O4B-C1B	4.56	1.47	1.41
2	C	300	CAA	P3B-O7A	4.58	1.66	1.51
2	C	300	CAA	O4B-C1B	4.65	1.47	1.41
2	F	300	CAA	C5A-C4A	4.91	1.51	1.40
2	C	300	CAA	C5A-C4A	5.02	1.51	1.40
2	F	300	CAA	C5P-N4P	5.53	1.46	1.33
2	C	300	CAA	C5P-N4P	5.64	1.46	1.33
2	F	300	CAA	C9P-N8P	7.26	1.48	1.33
2	C	300	CAA	C9P-N8P	7.45	1.49	1.33
2	C	300	CAA	C8A-N7A	9.83	1.53	1.34
2	F	300	CAA	C8A-N7A	9.89	1.53	1.34
2	F	300	CAA	C4A-N3A	9.89	1.50	1.35
2	C	300	CAA	C4A-N3A	10.02	1.50	1.35
2	F	300	CAA	C2A-N1A	11.11	1.55	1.33
2	C	300	CAA	C2A-N1A	11.20	1.55	1.33
2	C	300	CAA	C2A-N3A	11.38	1.52	1.32
2	F	300	CAA	C2A-N3A	11.64	1.52	1.32
2	C	300	CAA	O1-C1	12.95	1.41	1.21
2	F	300	CAA	O1-C1	13.47	1.42	1.21

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	300	CAA	O1-C1-S1P	-25.37	102.70	122.83
2	C	300	CAA	O1-C1-S1P	-18.88	107.85	122.83
2	F	300	CAA	N3A-C2A-N1A	-12.76	119.13	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	CAA	N3A-C2A-N1A	-12.61	119.24	128.89
2	C	300	CAA	C2-C1-S1P	-4.79	108.72	113.50
2	F	300	CAA	P2A-O3A-P1A	-3.97	121.59	132.73
2	F	300	CAA	C2-C1-S1P	-3.73	109.78	113.50
2	C	300	CAA	P2A-O3A-P1A	-3.36	123.30	132.73
2	F	300	CAA	O5P-C5P-N4P	-3.23	116.52	122.94
2	C	300	CAA	C4B-O4B-C1B	-2.37	107.12	109.72
2	F	300	CAA	C4B-O4B-C1B	-2.30	107.19	109.72
2	C	300	CAA	C2B-C1B-N9A	-2.26	110.84	114.29
2	C	300	CAA	C2P-C3P-N4P	-2.07	108.23	112.36
2	C	300	CAA	C3P-C2P-S1P	-2.01	105.97	111.36
2	F	300	CAA	C7P-C6P-C5P	2.03	115.66	112.31
2	F	300	CAA	C2P-S1P-C1	2.48	110.94	102.09
2	F	300	CAA	O3A-P2A-O6A	2.49	109.53	102.94
2	C	300	CAA	O3A-P2A-O6A	2.82	110.41	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	CAA	6	0
2	F	300	CAA	9	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<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	255/258 (98%)	0.20	9 (3%)	48 48	2, 2, 18, 46	0
1	B	255/258 (98%)	0.29	12 (4%)	35 36	2, 2, 18, 34	0
1	C	255/258 (98%)	0.13	10 (3%)	43 44	2, 2, 16, 33	0
1	D	255/258 (98%)	0.25	14 (5%)	29 29	2, 4, 24, 43	0
1	E	253/258 (98%)	0.33	14 (5%)	29 29	2, 5, 21, 45	0
1	F	254/258 (98%)	0.08	4 (1%)	74 74	2, 2, 15, 27	0
All	All	1527/1548 (98%)	0.21	63 (4%)	41 42	2, 2, 19, 46	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	HIS	5.3
1	E	2	THR	5.2
1	C	1	MET	4.3
1	B	237	GLU	4.1
1	D	254	PHE	4.1
1	E	4	GLU	4.1
1	E	3	TYR	3.8
1	E	24	ALA	3.8
1	D	255	THR	3.7
1	D	2	THR	3.6
1	C	245	ALA	3.3
1	F	247	ILE	3.3
1	F	72	ASP	3.2
1	F	251	ALA	3.1
1	A	73	LEU	3.1
1	D	247	ILE	3.1
1	A	253	GLN	3.0
1	A	247	ILE	2.8
1	D	248	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	72	ASP	2.8
1	B	184	ASP	2.7
1	A	251	ALA	2.7
1	D	48	ASP	2.7
1	B	22	PRO	2.6
1	D	253	GLN	2.6
1	F	244	ALA	2.6
1	B	253	GLN	2.5
1	E	42	GLU	2.5
1	C	181	PRO	2.4
1	B	12	GLN	2.4
1	E	23	GLN	2.4
1	E	124	THR	2.4
1	A	72	ASP	2.4
1	D	241	GLU	2.4
1	C	249	LYS	2.4
1	C	72	ASP	2.4
1	D	250	ARG	2.3
1	B	182	ALA	2.3
1	D	22	PRO	2.3
1	E	187	THR	2.3
1	B	183	ASP	2.3
1	B	47	PRO	2.3
1	A	183	ASP	2.3
1	C	104	TYR	2.3
1	D	251	ALA	2.2
1	E	12	GLN	2.2
1	C	237	GLU	2.2
1	B	0	SER	2.2
1	D	23	GLN	2.2
1	B	58	ALA	2.1
1	A	1	MET	2.1
1	C	253	GLN	2.1
1	B	68	LYS	2.1
1	E	123	ASP	2.1
1	E	25	LEU	2.1
1	E	182	ALA	2.1
1	C	159	ILE	2.1
1	E	185	LEU	2.1
1	A	23	GLN	2.1
1	A	255	THR	2.1
1	C	54	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	125	ALA	2.0
1	D	5	THR	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. 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
2	CAA	C	300	54/54	0.78	0.26	1.56	49,57,64,100	17
2	CAA	F	300	54/54	0.83	0.24	1.43	44,53,57,65	20

## 6.5 Other polymers [i](#)

There are no such residues in this entry.