



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2021 – 11:11 AM GMT

PDB ID : 7BDV  
Title : Structure of Can2 from *Sulfobacillus thermosulfidooxidans* in complex with cyclic tetra-adenylate (cA4)  
Authors : McQuarrie, S.; McMahon, S.A.; Gloster, T.M.; White, M.F.; Graham, S.; Zhu, W.; Gruschow, S.  
Deposited on : 2020-12-22  
Resolution : 2.02 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.17.1.dev1  
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) : 2.17.1.dev1

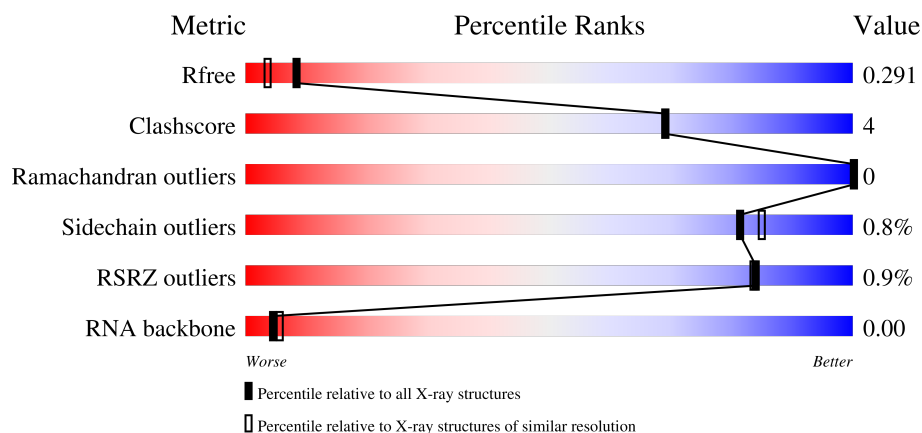
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)
RNA backbone	3102	1039 (2.50-1.54)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	366	<div> <div style="width: 90%;"></div> <div style="width: 7%;"></div> <div style="width: 3%;"></div> </div> 90% 7%
1	B	366	<div> <div style="width: 2%;"></div> <div style="width: 86%;"></div> <div style="width: 8%;"></div> <div style="width: 7%;"></div> </div> 2% 86% 8% 7%
1	C	366	<div> <div style="width: 0%;"></div> <div style="width: 85%;"></div> <div style="width: 7%;"></div> <div style="width: 7%;"></div> </div> 0% 85% 7% 7%
1	D	366	<div> <div style="width: 0%;"></div> <div style="width: 86%;"></div> <div style="width: 7%;"></div> <div style="width: 7%;"></div> </div> 0% 86% 7% 7%

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Mol	Chain	Length	Quality of chain
2	F	4	 50%50%
2	H	4	 25%75%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10989 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 Can2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	Se	0	0	0
			2748	1768	481	491	5	3			
1	B	342	Total	C	N	O	S	Se	0	0	2
			2553	1646	449	450	5	3			
1	C	341	Total	C	N	O	S	Se	0	2	0
			2641	1712	464	457	5	3			
1	D	341	Total	C	N	O	S	Se	0	1	1
			2598	1691	453	446	5	3			

- Molecule 2 is a RNA chain called cyclic tetra-adenylate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			
2	H	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			

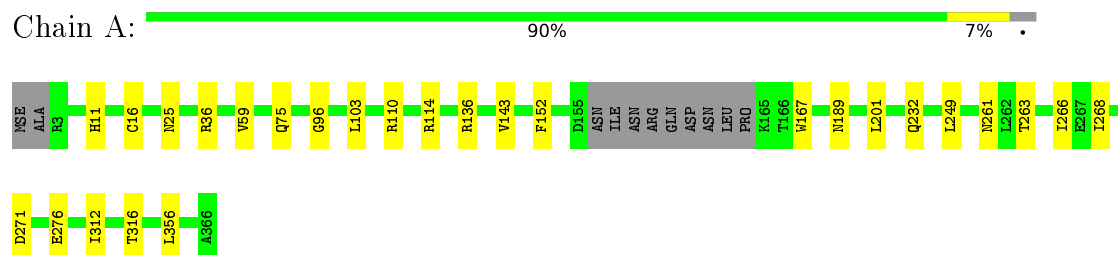
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	34	Total	O	0	1
			35	35		
3	C	60	Total	O	0	0
			60	60		
3	D	57	Total	O	0	0
			57	57		
3	F	10	Total	O	0	0
			10	10		
3	H	8	Total	O	0	0
			8	8		

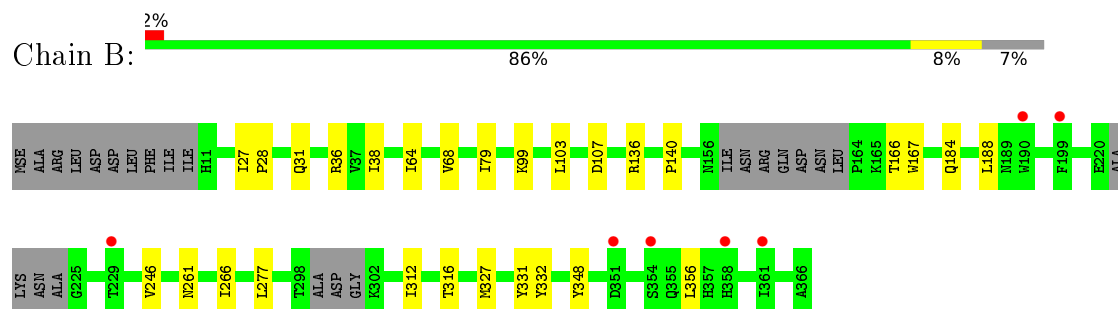
### 3 Residue-property plots [i](#)

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.

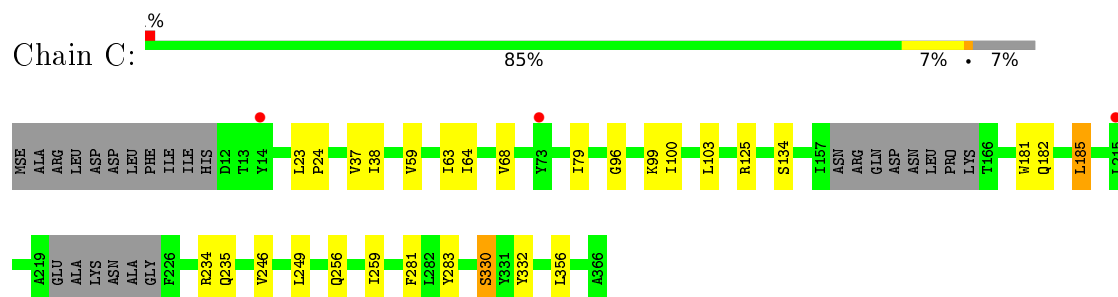
#### • Molecule 1: Can2



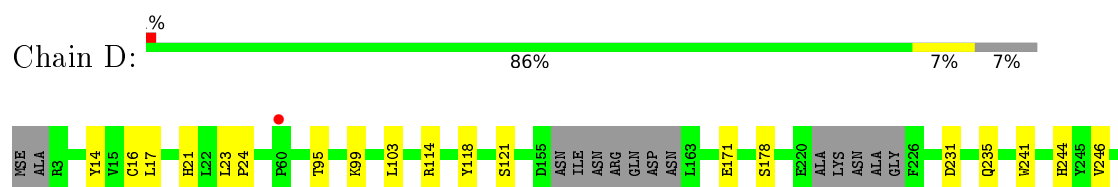
#### • Molecule 1: Can2

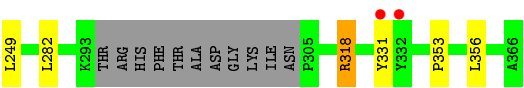


#### • Molecule 1: Can2



#### • Molecule 1: Can2





- Molecule 2: cyclic tetra-adenylate



- Molecule 2: cyclic tetra-adenylate



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.86Å 85.97Å 237.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.37 – 2.02 51.32 – 2.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.37-2.02) 100.0 (51.32-2.02)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.241 , 0.290 0.245 , 0.291	Depositor DCC
$R_{free}$ test set	5122 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.70	0/2810	0.80	0/3823
1	B	0.67	0/2608	0.76	0/3537
1	C	0.69	0/2707	0.80	0/3678
1	D	0.68	0/2663	0.78	0/3621
2	F	1.45	1/99 (1.0%)	3.12	12/152 (7.9%)
2	H	0.98	0/99	1.92	4/152 (2.6%)
All	All	0.70	1/10986 (0.0%)	0.86	16/14963 (0.1%)

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
2	F	1	0
2	H	1	0
All	All	2	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	A	C3'-O3'	-6.58	1.32	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	A	C3'-C2'-C1'	-18.54	86.67	101.50
2	F	4	A	O5'-P-OP1	-11.07	95.74	105.70
2	F	3	A	O3'-P-O5'	-10.18	84.67	104.00
2	H	1	A	C3'-C2'-C1'	-9.89	93.58	101.50
2	F	3	A	C4'-C3'-O3'	9.24	131.49	113.00
2	F	4	A	OP1-P-OP2	8.81	132.81	119.60
2	F	3	A	O4'-C4'-C3'	-8.64	95.36	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	A	OP1-P-O3'	7.53	121.76	105.20
2	F	3	A	C4'-C3'-C2'	-6.79	95.81	102.60
2	F	1	A	OP1-P-OP2	-6.68	109.57	119.60
2	H	1	A	OP2-P-O3'	6.10	118.62	105.20
2	H	1	A	N9-C1'-C2'	5.63	121.31	114.00
2	F	1	A	OP2-P-O3'	5.25	116.76	105.20
2	F	3	A	N9-C1'-C2'	5.25	120.83	114.00
2	F	3	A	C8-N9-C4	5.24	107.89	105.80
2	H	4	A	C3'-C2'-C1'	-5.08	97.44	101.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	3	A	C3'
2	H	1	A	C3'

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	2748	0	2599	19	0
1	B	2553	0	2325	18	0
1	C	2641	0	2528	22	0
1	D	2598	0	2421	26	0
2	F	88	0	44	0	0
2	H	88	0	44	2	0
3	A	103	0	0	1	0
3	B	35	0	0	0	0
3	C	60	0	0	1	0
3	D	57	0	0	1	0
3	F	10	0	0	0	0
3	H	8	0	0	0	0
All	All	10989	0	9961	76	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 (76) 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:D:14:TYR:CE2	1:D:16:CYS:SG	2.72	0.82
1:D:121:SER:OG	2:H:2:A:C2	2.34	0.79
1:A:103:LEU:HD23	1:B:103:LEU:HD23	1.72	0.70
1:D:246:VAL:HG22	1:D:356:LEU:HD21	1.74	0.69
1:C:103:LEU:HD23	1:D:103:LEU:HD23	1.74	0.69
1:A:59:VAL:HG12	1:A:59:VAL:O	1.94	0.67
1:C:59:VAL:HG12	1:C:59:VAL:O	2.01	0.61
1:C:100:ILE:HD11	1:D:118:TYR:CG	2.36	0.61
1:C:235[B]:GLN:NE2	1:C:235[B]:GLN:HA	2.16	0.59
1:A:16:CYS:HB2	1:A:25:ASN:ND2	2.19	0.57
1:C:99:LYS:NZ	1:D:95:THR:O	2.34	0.57
1:D:171:GLU:OE2	1:D:244:HIS:ND1	2.39	0.56
1:C:100:ILE:HD11	1:D:118:TYR:CD1	2.41	0.55
1:B:38:ILE:HD13	1:B:64:ILE:HB	1.89	0.54
1:C:246:VAL:HG22	1:C:356:LEU:HD21	1.88	0.54
1:B:31:GLN:HG3	1:B:140:PRO:HG3	1.91	0.53
1:D:331:TYR:CD1	1:D:353:PRO:HG2	2.44	0.53
1:C:181:TRP:HB3	1:C:185:LEU:HD22	1.91	0.52
1:B:38:ILE:CD1	1:B:64:ILE:HD12	2.39	0.52
1:D:318:ARG:CG	1:D:318:ARG:HH21	2.23	0.52
1:D:178:SER:HB3	1:D:331:TYR:CE1	2.45	0.52
1:A:249:LEU:HD12	1:A:356:LEU:HD23	1.91	0.51
1:B:246:VAL:HG22	1:B:356:LEU:HD11	1.92	0.51
1:C:256:GLN:HB2	3:C:406:HOH:O	2.10	0.51
1:C:38:ILE:HD13	1:C:64:ILE:HB	1.91	0.51
1:C:249:LEU:HD12	1:C:356:LEU:HD23	1.93	0.50
1:C:182:GLN:HG2	1:C:332:TYR:CE1	2.48	0.49
1:A:152:PHE:CD1	1:A:268:ILE:HG22	2.47	0.49
1:C:96:GLY:O	1:D:99:LYS:HE2	2.12	0.49
1:C:259:ILE:HD13	1:C:283:TYR:CD1	2.48	0.48
1:C:234:ARG:NH2	1:C:235[B]:GLN:OE1	2.47	0.48
1:D:178:SER:CB	1:D:331:TYR:CE1	2.97	0.47
1:D:244:HIS:HB2	3:D:450:HOH:O	2.13	0.47
1:B:312:ILE:O	1:B:316:THR:HG22	2.15	0.47
1:A:136:ARG:HH11	1:A:136:ARG:HG3	1.78	0.47
1:B:184:GLN:O	1:B:188:LEU:HD13	2.15	0.47
1:B:327:MSE:HE3	1:B:348:TYR:CD2	2.50	0.46
1:B:331:TYR:CG	1:B:332:TYR:CZ	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:MSE:HE3	1:B:348:TYR:HD2	1.79	0.46
1:D:114:ARG:NE	1:D:114:ARG:HA	2.31	0.46
1:D:241:TRP:CH2	1:D:331:TYR:CD1	3.03	0.46
1:A:263:THR:HG21	1:A:266:ILE:HG22	1.98	0.46
1:D:171:GLU:OE2	1:D:244:HIS:HB3	2.16	0.45
1:B:266:ILE:CG1	1:B:277:LEU:HB2	2.46	0.45
1:D:282:LEU:HD12	1:D:282:LEU:HA	1.83	0.45
1:A:312:ILE:O	1:A:316:THR:HG23	2.16	0.45
1:C:330:SER:OG	1:C:332:TYR:O	2.33	0.45
1:B:68:VAL:HG12	1:B:79:ILE:HG13	1.99	0.44
1:A:167:TRP:CH2	1:A:232:GLN:HG3	2.52	0.44
1:A:75:GLN:OE1	1:A:75:GLN:N	2.49	0.44
1:B:136:ARG:HG3	1:B:136:ARG:HH11	1.82	0.44
1:A:110:ARG:NH1	1:B:107:ASP:OD1	2.51	0.44
1:A:271:ASP:HB2	3:A:468:HOH:O	2.17	0.44
1:B:166:THR:HG23	1:B:167:TRP:CD1	2.52	0.44
1:C:37:VAL:HB	1:C:63:ILE:HD13	1.99	0.43
1:D:331:TYR:HA	1:D:353:PRO:HG3	1.99	0.43
1:A:263:THR:CG2	1:A:266:ILE:CG2	2.96	0.43
1:D:23:LEU:N	1:D:24:PRO:HD2	2.33	0.43
1:C:100:ILE:CD1	1:D:118:TYR:CD1	3.01	0.43
1:A:143:VAL:HG23	1:A:261:ASN:HB2	2.00	0.43
1:A:11:HIS:ND1	1:A:114:ARG:NH2	2.67	0.42
1:A:96:GLY:O	1:B:99:LYS:HE2	2.18	0.42
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.94	0.41
1:C:125:ARG:NH1	1:C:134:SER:OG	2.54	0.41
1:D:318:ARG:HH21	1:D:318:ARG:HG2	1.86	0.41
1:D:17:LEU:N	1:D:17:LEU:HD12	2.36	0.41
1:D:249:LEU:HD12	1:D:356:LEU:HD23	2.03	0.41
1:C:23:LEU:N	1:C:24:PRO:HD2	2.36	0.40
1:D:21:HIS:HD2	2:H:2:A:OP1	2.04	0.40
1:D:231:ASP:OD2	1:D:235:GLN:NE2	2.54	0.40
1:C:68:VAL:HG12	1:C:79:ILE:HG13	2.02	0.40
1:C:259:ILE:HD12	1:C:281:PHE:CD2	2.56	0.40
1:B:27:ILE:HB	1:B:28:PRO:HD3	2.03	0.40
1:A:167:TRP:HH2	1:A:232:GLN:HG3	1.86	0.40
1:A:263:THR:CG2	1:A:266:ILE:HG22	2.52	0.40
1:B:38:ILE:HD11	1:B:64:ILE:HD12	2.02	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	351/366 (96%)	348 (99%)	3 (1%)	0	100	100
1	B	333/366 (91%)	328 (98%)	5 (2%)	0	100	100
1	C	337/366 (92%)	333 (99%)	4 (1%)	0	100	100
1	D	334/366 (91%)	331 (99%)	3 (1%)	0	100	100
All	All	1355/1464 (93%)	1340 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/324 (83%)	265 (99%)	3 (1%)	73	77
1	B	231/324 (71%)	229 (99%)	2 (1%)	78	82
1	C	258/324 (80%)	256 (99%)	2 (1%)	81	85
1	D	240/324 (74%)	239 (100%)	1 (0%)	91	93
All	All	997/1296 (77%)	989 (99%)	8 (1%)	81	85

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

Mol	Chain	Res	Type
1	A	36	ARG
1	A	189	ASN

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Mol	Chain	Res	Type
1	A	276	GLU
1	B	36	ARG
1	B	261	ASN
1	C	185	LEU
1	C	330	SER
1	D	318	ARG

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	F	3/4 (75%)	3 (100%)	1 (33%)
2	H	4/4 (100%)	3 (75%)	1 (25%)
All	All	7/8 (87%)	6 (85%)	2 (28%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	2	A
2	F	3	A
2	F	4	A
2	H	2	A
2	H	3	A
2	H	4	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	F	3	A
2	H	1	A

## 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	352/366 (96%)	0.08	0 100 100	28, 44, 63, 95	0
1	B	339/366 (92%)	0.20	7 (2%) 63 63	31, 59, 84, 103	0
1	C	338/366 (92%)	0.08	3 (0%) 84 83	29, 50, 74, 98	0
1	D	338/366 (92%)	0.14	3 (0%) 84 83	35, 55, 80, 109	0
2	F	4/4 (100%)	-0.74	0 100 100	31, 32, 35, 36	0
2	H	4/4 (100%)	-0.69	0 100 100	39, 41, 43, 45	0
All	All	1375/1472 (93%)	0.12	13 (0%) 84 83	28, 51, 78, 109	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	LEU	2.7
1	D	60	PRO	2.5
1	D	331	TYR	2.5
1	B	354	SER	2.4
1	B	361	ILE	2.4
1	B	358	HIS	2.3
1	B	229	THR	2.3
1	B	351	ASP	2.2
1	B	190	TRP	2.2
1	D	332	TYR	2.2
1	C	14	TYR	2.0
1	B	199	PHE	2.0
1	C	73	TYR	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.