



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:45 AM GMT

PDB ID : 3CDK  
Title : Crystal structure of the co-expressed succinyl-CoA transferase A and B complex from *Bacillus subtilis*  
Authors : Kim, Y.; Zhou, M.; Stols, L.; Eschenfeldt, W.; Donnelly, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2008-02-27  
Resolution : 2.59 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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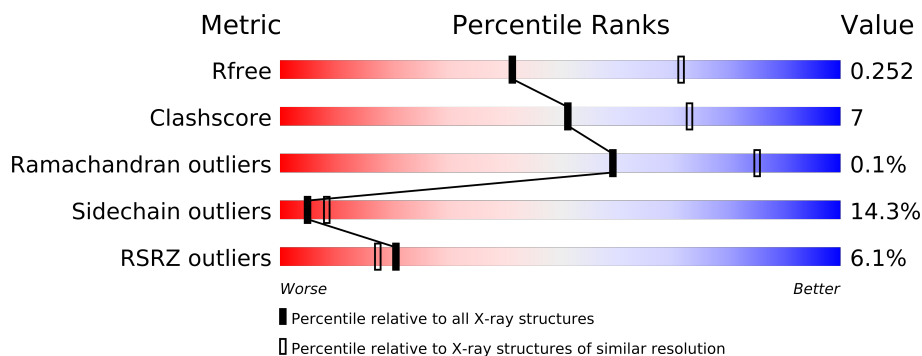
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.59 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	241	
1	C	241	
2	B	219	
2	D	219	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6720 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Succinyl-CoA:3-ketoacid-coenzymeA transferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	3	0
			1752	1104	309	334	5			
1	C	229	Total	C	N	O	S	0	0	0
			1725	1090	302	327	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P42315
A	1	ASN	-	EXPRESSION TAG	UNP P42315
A	2	ALA	-	EXPRESSION TAG	UNP P42315
C	0	SER	-	EXPRESSION TAG	UNP P42315
C	1	ASN	-	EXPRESSION TAG	UNP P42315
C	2	ALA	-	EXPRESSION TAG	UNP P42315

- Molecule 2 is a protein called Succinyl-CoA:3-ketoacid-coenzymeA transferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	2	0
			1613	1008	276	316	13			
2	D	200	Total	C	N	O	S	0	1	0
			1515	951	256	295	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	EXPRESSION TAG	UNP P42316
B	-1	ASN	-	EXPRESSION TAG	UNP P42316
B	0	ALA	-	EXPRESSION TAG	UNP P42316
D	-2	SER	-	EXPRESSION TAG	UNP P42316
D	-1	ASN	-	EXPRESSION TAG	UNP P42316
D	0	ALA	-	EXPRESSION TAG	UNP P42316

- Molecule 3 is water.

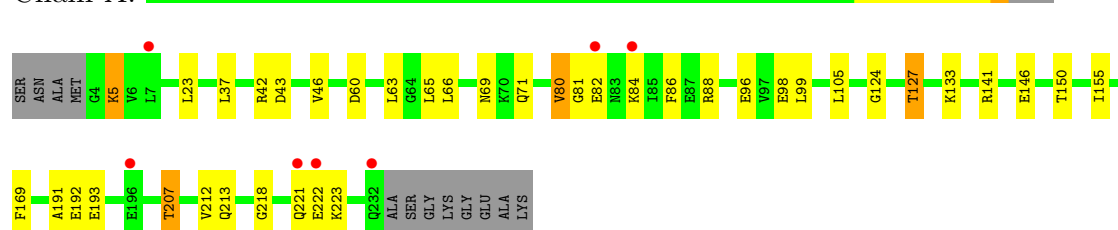
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total 48	O 48	0	0
3	B	26	Total 26	O 26	0	0
3	C	27	Total 27	O 27	0	0
3	D	14	Total 14	O 14	0	0

### 3 Residue-property plots

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.

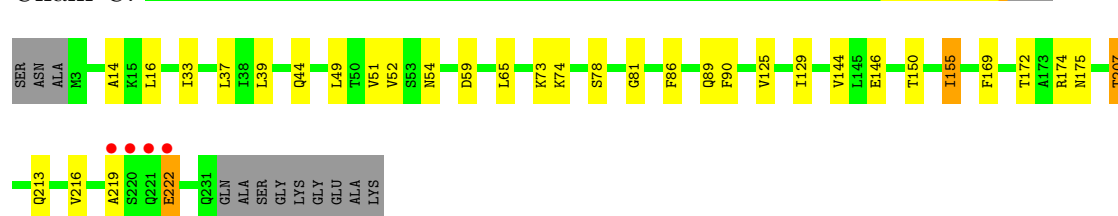
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzymeA transferase subunit A

Chain A:



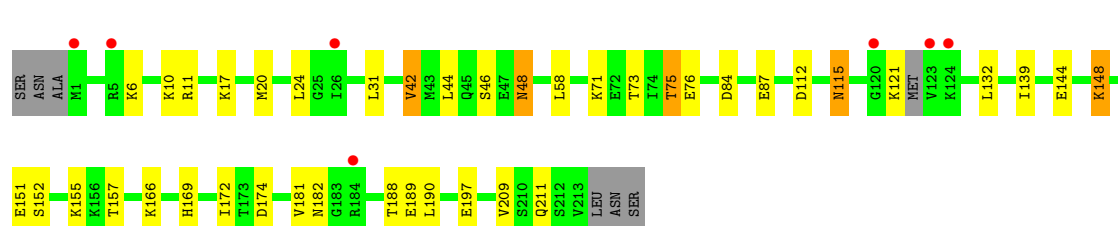
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzymeA transferase subunit A

Chain C:



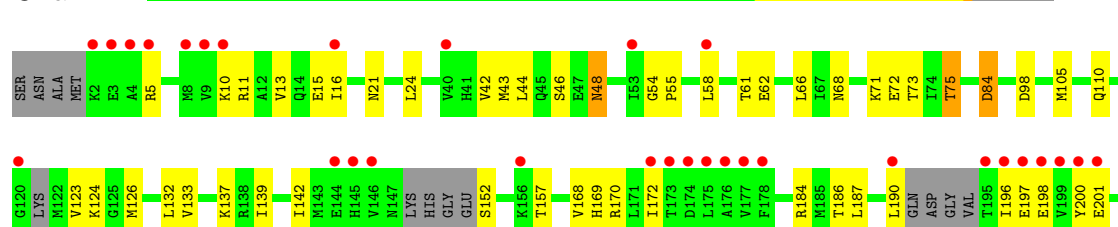
- Molecule 2: Succinyl-CoA:3-ketoacid-coenzymeA transferase subunit B

Chain B:



- Molecule 2: Succinyl-CoA:3-ketoacid-coenzymeA transferase subunit B

Chain D:



A205	D206	F207	A208	V209	S210	GLN	SER	VAL	LEU	ASN	SER
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.34Å 70.40Å 98.00Å 90.00° 106.31° 90.00°	Depositor
Resolution (Å)	48.30 – 2.59 48.30 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.30-2.59) 99.2 (48.30-2.59)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.193 , 0.253 0.194 , 0.252	Depositor DCC
$R_{free}$ test set	1417 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28070 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.79	2/1777 (0.1%)	0.81	0/2395
1	C	0.76	3/1750 (0.2%)	0.80	2/2359 (0.1%)
2	B	0.69	0/1632	0.78	0/2197
2	D	0.98	8/1531 (0.5%)	0.74	1/2059 (0.0%)
All	All	0.81	13/6690 (0.2%)	0.79	3/9010 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	198	GLU	CD-OE2	23.59	1.51	1.25
2	D	201	GLU	CG-CD	8.08	1.64	1.51
2	D	190	LEU	C-O	7.88	1.38	1.23
2	D	201	GLU	CD-OE2	7.28	1.33	1.25
2	D	201	GLU	CD-OE1	7.08	1.33	1.25
1	C	222	GLU	CD-OE2	6.13	1.32	1.25
2	D	197	GLU	CD-OE1	5.88	1.32	1.25
2	D	152	SER	CB-OG	5.41	1.49	1.42
1	A	98	GLU	CG-CD	5.35	1.59	1.51
2	D	198	GLU	CD-OE1	-5.33	1.19	1.25
1	C	222	GLU	CG-CD	5.24	1.59	1.51
1	C	146	GLU	CG-CD	5.20	1.59	1.51
1	A	222	GLU	CB-CG	5.12	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ARG	CB-CG-CD	-5.71	96.75	111.60
1	C	155	ILE	N-CA-C	-5.31	96.65	111.00
2	D	84	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1752	0	0	15	0
1	C	1725	0	0	7	0
2	B	1613	0	0	10	0
2	D	1515	0	0	18	0
3	A	48	0	0	2	0
3	B	26	0	0	0	0
3	C	27	0	0	1	0
3	D	14	0	0	0	0
All	All	6720	0	0	48	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:LEU:CB	3:A:253:HOH:O	2.21	0.87
2:D:200:TYR:CD1	2:D:207:PHE:CE1	2.72	0.77
2:D:15:GLU:OE2	2:D:170:ARG:NH1	2.19	0.74
2:D:139:ILE:N	2:D:169:HIS:CD2	2.58	0.72
1:C:73:LYS:NZ	3:C:257:HOH:O	2.24	0.71
2:B:75:THR:CG2	2:B:76:GLU:N	2.55	0.69
2:D:13:VAL:O	2:D:16:ILE:CG2	2.41	0.69
2:D:200:TYR:CE1	2:D:207:PHE:CE1	2.86	0.64
2:D:16:ILE:CG2	2:D:16:ILE:O	2.44	0.64
2:B:11:ARG:NH1	2:B:189:GLU:OE2	2.33	0.62
2:B:115:ASN:ND2	2:B:115:ASN:C	2.52	0.62
1:A:80:VAL:CG2	1:A:86:PHE:CZ	2.84	0.61
2:D:200:TYR:CD1	2:D:207:PHE:CZ	2.90	0.60
2:D:68:ASN:ND2	2:D:72:GLU:OE1	2.35	0.60
1:C:169:PHE:CE2	1:C:207:THR:CG2	2.85	0.59
1:C:54:ASN:ND2	1:C:78:SER:OG	2.35	0.59
2:D:21:ASN:N	2:D:98:ASP:OD2	2.36	0.58
2:D:186:THR:CG2	2:D:208:ALA:O	2.51	0.58
1:A:42[B]:ARG:CG	1:A:42[B]:ARG:NH2	2.66	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:69:ASN:ND2	1:A:71:GLN:OE1	2.38	0.57
2:B:48:ASN:ND2	2:B:48:ASN:N	2.52	0.57
2:B:46:SER:OG	2:B:48:ASN:ND2	2.39	0.55
2:B:148:LYS:CD	2:B:148:LYS:N	2.70	0.55
2:D:42:VAL:CG1	2:D:43:MET:N	2.71	0.53
1:A:192:GLU:OE2	1:A:223:LYS:NZ	2.41	0.53
2:D:48:ASN:ND2	2:D:48:ASN:N	2.58	0.51
1:A:42[B]:ARG:NH2	1:A:43:ASP:OD1	2.44	0.51
1:A:5:LYS:CE	1:A:212:VAL:O	2.59	0.51
2:B:174:ASP:N	2:B:174:ASP:OD1	2.45	0.50
2:D:55:PRO:O	2:D:75:THR:CB	2.61	0.48
1:A:169:PHE:CE1	1:A:207:THR:CG2	2.96	0.48
1:A:80:VAL:CG2	1:A:86:PHE:CE1	2.97	0.47
1:A:80:VAL:CG1	1:A:81:GLY:N	2.76	0.47
2:D:11:ARG:NH2	2:D:11:ARG:O	2.48	0.45
1:C:90:PHE:CE2	2:D:123:VAL:CG1	2.99	0.45
1:A:191:ALA:O	1:A:218:GLY:N	2.51	0.44
1:A:124:GLY:O	1:A:127:THR:CB	2.67	0.43
2:D:54:GLY:N	2:D:75:THR:O	2.52	0.43
1:A:42[A]:ARG:NH2	1:A:65:LEU:O	2.52	0.42
2:D:46:SER:OG	2:D:48:ASN:ND2	2.52	0.42
2:B:20:MET:O	2:B:42:VAL:CG2	2.67	0.42
2:B:139:ILE:N	2:B:169:HIS:ND1	2.67	0.41
1:C:219:ALA:CB	1:C:222:GLU:OE1	2.68	0.41
1:C:14:ALA:C	1:C:16:LEU:N	2.73	0.41
1:A:221:GLN:CG	3:A:287:HOH:O	2.68	0.41
1:A:133:LYS:NZ	1:A:146:GLU:OE2	2.54	0.41
2:B:112:ASP:OD1	2:B:166:LYS:N	2.54	0.40
1:C:81:GLY:O	2:D:124:LYS:NZ	2.55	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	230/241 (95%)	216 (94%)	14 (6%)	0	100	100
1	C	227/241 (94%)	216 (95%)	10 (4%)	1 (0%)	43	72
2	B	210/219 (96%)	198 (94%)	12 (6%)	0	100	100
2	D	193/219 (88%)	182 (94%)	11 (6%)	0	100	100
All	All	860/920 (94%)	812 (94%)	47 (6%)	1 (0%)	59	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	175	ASN

### 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	182/186 (98%)	161 (88%)	21 (12%)	8	15
1	C	179/186 (96%)	158 (88%)	21 (12%)	8	14
2	B	175/179 (98%)	144 (82%)	31 (18%)	3	4
2	D	164/179 (92%)	137 (84%)	27 (16%)	3	5
All	All	700/730 (96%)	600 (86%)	100 (14%)	5	8

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	23	LEU
1	A	37	LEU
1	A	46	VAL
1	A	60	ASP
1	A	63	LEU
1	A	66	LEU
1	A	80	VAL
1	A	82	GLU
1	A	84	LYS
1	A	88	ARG

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Mol	Chain	Res	Type
1	A	96[A]	GLU
1	A	96[B]	GLU
1	A	99	LEU
1	A	127	THR
1	A	141	ARG
1	A	150	THR
1	A	155	ILE
1	A	193	GLU
1	A	207	THR
1	A	213	GLN
2	B	6	LYS
2	B	10	LYS
2	B	17	LYS
2	B	24	LEU
2	B	31	LEU
2	B	42	VAL
2	B	44	LEU
2	B	48	ASN
2	B	58	LEU
2	B	71	LYS
2	B	73	THR
2	B	75	THR
2	B	84	ASP
2	B	87	GLU
2	B	115	ASN
2	B	121	LYS
2	B	132	LEU
2	B	144	GLU
2	B	148	LYS
2	B	151	GLU
2	B	152	SER
2	B	155	LYS
2	B	157	THR
2	B	172	ILE
2	B	181	VAL
2	B	182	ASN
2	B	188	THR
2	B	190	LEU
2	B	197	GLU
2	B	209	VAL
2	B	211	GLN
1	C	33	ILE

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Mol	Chain	Res	Type
1	C	37	LEU
1	C	39	LEU
1	C	44	GLN
1	C	49	LEU
1	C	51	VAL
1	C	52	VAL
1	C	59	ASP
1	C	65	LEU
1	C	74	LYS
1	C	86	PHE
1	C	89	GLN
1	C	125	VAL
1	C	129	ILE
1	C	144	VAL
1	C	150	THR
1	C	155	ILE
1	C	172	THR
1	C	207	THR
1	C	213	GLN
1	C	216	VAL
2	D	5	ARG
2	D	10	LYS
2	D	24	LEU
2	D	44	LEU
2	D	48	ASN
2	D	58	LEU
2	D	61	THR
2	D	62	GLU
2	D	66	LEU
2	D	71	LYS
2	D	73	THR
2	D	75	THR
2	D	84	ASP
2	D	105	MET
2	D	110	GLN
2	D	126	MET
2	D	132	LEU
2	D	133	VAL
2	D	137	LYS
2	D	142	ILE
2	D	157	THR
2	D	168	VAL

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Mol	Chain	Res	Type
2	D	172	ILE
2	D	184	ARG
2	D	187	LEU
2	D	196	ILE
2	D	206	ASP

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	229/241 (95%)	0.04	7 (3%) 47 43	22, 38, 71, 117	0
1	C	229/241 (95%)	0.01	4 (1%) 67 66	23, 44, 73, 131	0
2	B	212/219 (96%)	0.09	7 (3%) 44 41	24, 45, 74, 97	0
2	D	200/219 (91%)	0.88	35 (17%) 2 1	30, 74, 140, 181	0
All	All	870/920 (94%)	0.24	53 (6%) 21 17	22, 47, 106, 181	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	199	VAL	8.7
2	D	201	GLU	8.4
2	D	178	PHE	7.4
2	D	197	GLU	5.7
2	D	4	ALA	5.7
2	D	200	TYR	5.6
2	D	195	THR	5.5
2	D	175	LEU	5.5
2	D	196	ILE	4.7
2	D	5	ARG	4.6
1	C	219	ALA	4.3
2	D	173	THR	4.3
2	B	123	VAL	4.3
1	C	221	GLN	4.2
2	D	207	PHE	4.1
2	D	172	ILE	4.1
2	B	1	MET	4.1
1	A	232	GLN	3.9
1	C	220	SER	3.9
2	D	190	LEU	3.9
2	D	10	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	16	ILE	3.4
2	D	145	HIS	3.2
2	B	124	LYS	3.2
2	D	58	LEU	3.2
2	D	2	LYS	3.0
1	A	7	LEU	2.9
1	A	84	LYS	2.9
2	D	40	VAL	2.8
2	D	174	ASP	2.8
2	D	206	ASP	2.7
2	D	9	VAL	2.6
1	C	222	GLU	2.5
2	D	8	MET	2.5
2	D	156	LYS	2.5
1	A	222	GLU	2.5
2	D	3	GLU	2.5
2	D	176	ALA	2.5
1	A	196	GLU	2.4
2	D	144	GLU	2.4
2	D	198	GLU	2.3
2	D	146	VAL	2.3
2	D	53	ILE	2.3
2	D	177	VAL	2.2
1	A	221	GLN	2.2
2	B	120	GLY	2.2
2	D	205	ALA	2.1
2	B	5	ARG	2.1
2	D	210	SER	2.1
2	B	26	ILE	2.1
1	A	82	GLU	2.0
2	D	120	GLY	2.0
2	B	184	ARG	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 ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.