



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 02:30 AM BST

PDB ID : 6WAN  
Title : Structure of Acinetobacter baumannii Cap4 SAVED/CARF-domain containing receptor with the cyclic trinucleotide 3'3'3'-cAAA  
Authors : Lowey, B.; Whiteley, A.T.; Keszei, A.F.A.; Morehouse, B.R.; Antine, S.P.; Cabrera, V.; Schwede, F.; Mekalanos, J.J.; Shao, S.; Lee, A.S.Y.; Kranzusch, P.J.  
Deposited on : 2020-03-25  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.13.1  
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) : 2.13.1

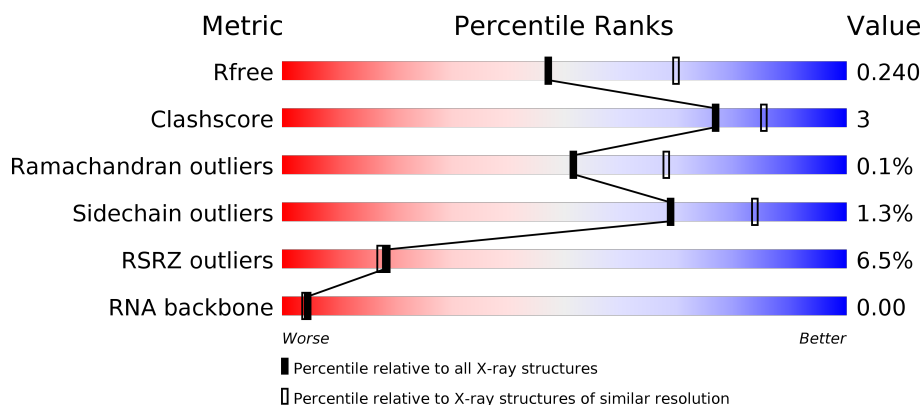
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 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	462	<div> <div>4%</div> <div>87% 8% 5%</div> </div>
1	B	462	<div> <div>4%</div> <div>87% 7% 5%</div> </div>
1	C	462	<div> <div>7%</div> <div>88% 6% 5%</div> </div>
1	D	462	<div> <div>8%</div> <div>85% 9% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	462	
1	F	462	
2	G	3	
2	H	3	
2	I	3	
2	J	3	
2	K	3	
2	L	3	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21812 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 SAVED domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3518	2245	593	669	11			
1	B	438	Total	C	N	O	S	0	0	0
			3518	2245	593	669	11			
1	C	438	Total	C	N	O	S	0	0	0
			3518	2245	593	669	11			
1	D	435	Total	C	N	O	S	0	0	0
			3489	2223	590	665	11			
1	E	437	Total	C	N	O	S	0	0	0
			3513	2242	592	668	11			
1	F	415	Total	C	N	O	S	0	0	0
			3338	2129	563	636	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP C0VHC9
B	1	SER	-	expression tag	UNP C0VHC9
C	1	SER	-	expression tag	UNP C0VHC9
D	1	SER	-	expression tag	UNP C0VHC9
E	1	SER	-	expression tag	UNP C0VHC9
F	1	SER	-	expression tag	UNP C0VHC9

- Molecule 2 is a RNA chain called Cyclic RNA (R(P\*AP\*AP\*A)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	H	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	I	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	K	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			
2	L	3	Total	C	N	O	P	0	0	0
			66	30	15	18	3			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

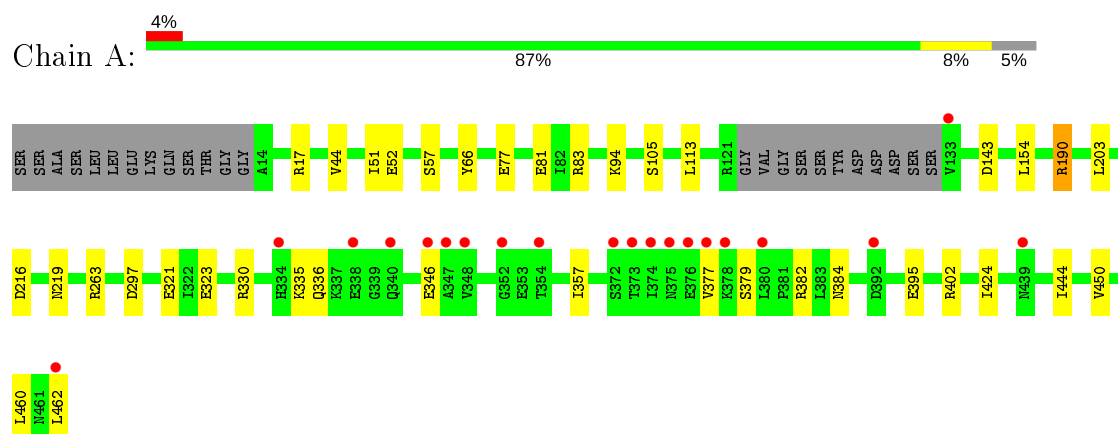
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total 84	O 84	0	0
4	B	76	Total 76	O 76	0	0
4	C	90	Total 90	O 90	0	0
4	D	83	Total 83	O 83	0	0
4	E	81	Total 81	O 81	0	0
4	F	71	Total 71	O 71	0	0
4	H	1	Total 1	O 1	0	0
4	J	2	Total 2	O 2	0	0
4	K	3	Total 3	O 3	0	0
4	L	1	Total 1	O 1	0	0

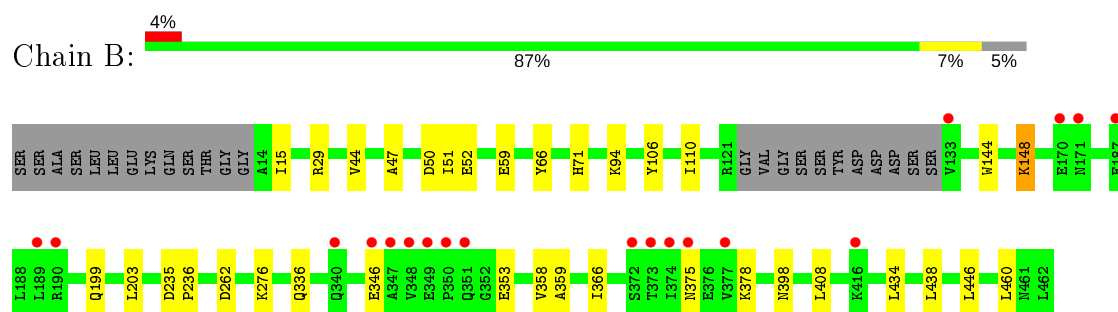
### 3 Residue-property plots [i](#)

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.

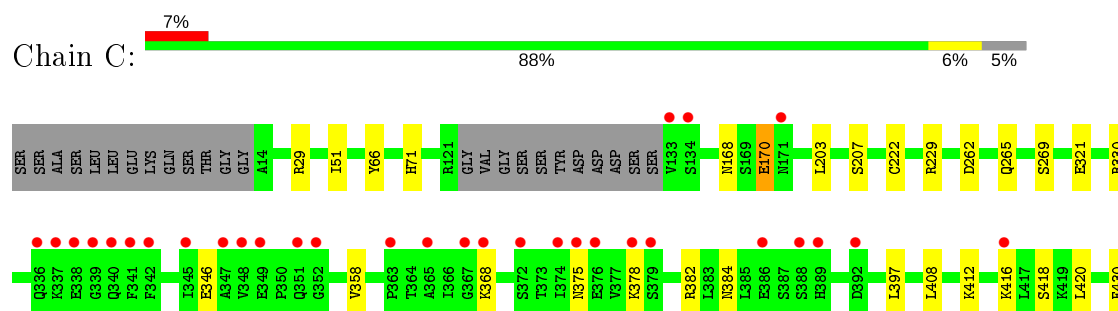
- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein

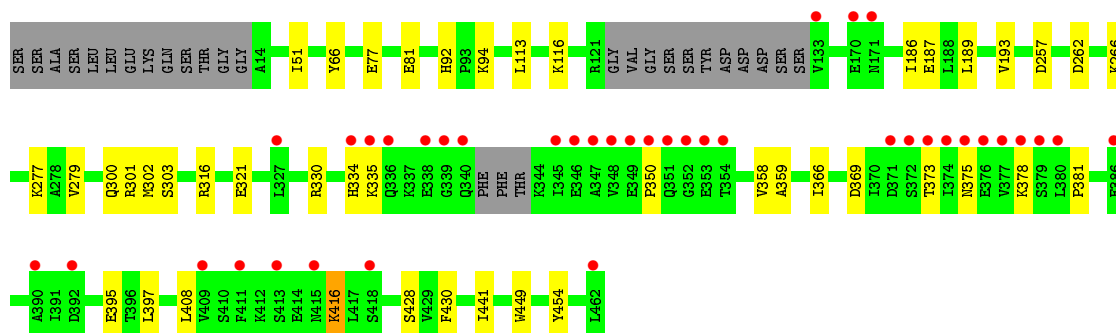
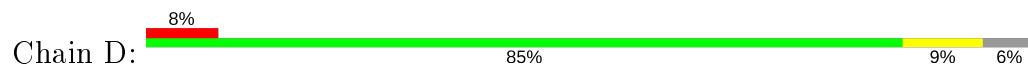


- Molecule 1: SAVED domain-containing protein

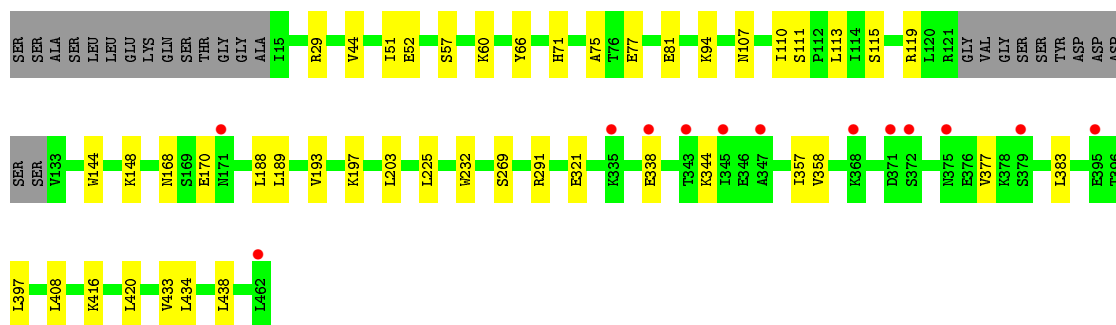
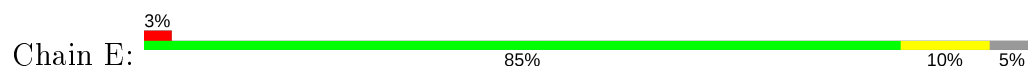




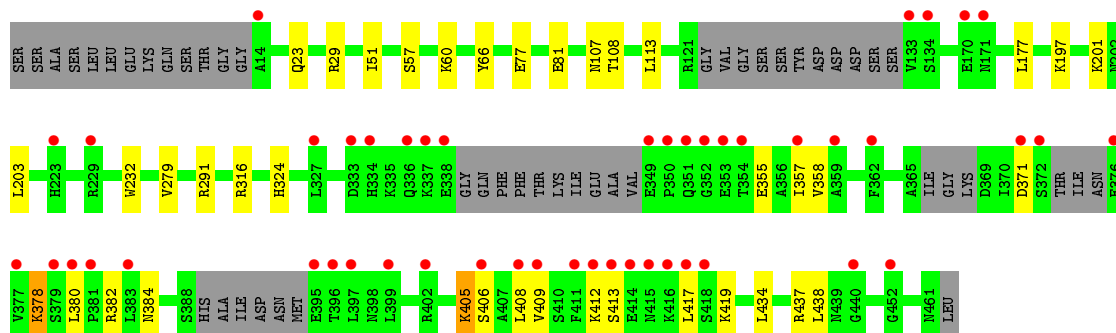
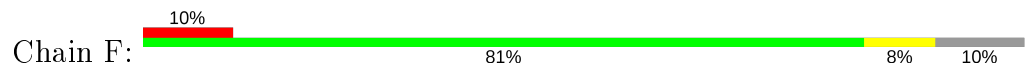
- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein



- Molecule 1: SAVED domain-containing protein



- Molecule 2: Cyclic RNA (R(P\*AP\*AP\*A))







- Molecule 2: Cyclic RNA (R(P\*AP\*AP\*A))

Chain H: 33% 33% 33%

A horizontal bar divided into three equal segments of yellow, orange, and red, each labeled with 33%.



- Molecule 2: Cyclic RNA (R(P\*AP\*AP\*A))

Chain I: 33% 67%

A horizontal bar divided into two segments: a yellow segment on the left labeled 33%, and an orange segment on the right labeled 67%.



- Molecule 2: Cyclic RNA (R(P\*AP\*AP\*A))

Chain J: 33% 67%

A horizontal bar divided into two segments: a yellow segment on the left labeled 33%, and a red segment on the right labeled 67%.



- Molecule 2: Cyclic RNA (R(P\*AP\*AP\*A))

Chain K: 33% 33% 33%

A horizontal bar divided into three equal segments of yellow, orange, and red, each labeled with 33%.



- Molecule 2: Cyclic RNA (R(P\*AP\*AP\*A))

Chain L: 33% 67%

A horizontal bar divided into two segments: a yellow segment on the left labeled 33%, and an orange segment on the right labeled 67%.



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.50Å 111.18Å 163.75Å 90.00° 100.36° 90.00°	Depositor
Resolution (Å)	38.80 – 2.40 38.80 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.80-2.40) 91.5 (38.80-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.69 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.208 , 0.240 0.208 , 0.240	Depositor DCC
$R_{free}$ test set	2000 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 ⓘ

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	0.25	0/3593	0.41	0/4856
1	B	0.24	0/3593	0.42	0/4856
1	C	0.25	0/3593	0.42	0/4856
1	D	0.24	0/3561	0.42	0/4811
1	E	0.24	0/3588	0.41	0/4849
1	F	0.24	0/3406	0.42	0/4599
2	G	7.33	34/74 (45.9%)	7.50	35/113 (31.0%)
2	H	7.33	34/74 (45.9%)	7.51	34/113 (30.1%)
2	I	7.27	34/74 (45.9%)	7.68	38/113 (33.6%)
2	J	7.34	34/74 (45.9%)	7.85	38/113 (33.6%)
2	K	7.22	32/74 (43.2%)	7.60	33/113 (29.2%)
2	L	7.32	34/74 (45.9%)	7.86	35/113 (31.0%)
All	All	1.07	202/21778 (0.9%)	1.23	213/29505 (0.7%)

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	A	N7-C5	21.29	1.52	1.39
2	L	1	A	N7-C5	20.93	1.51	1.39
2	J	1	A	N7-C5	20.61	1.51	1.39
2	H	1	A	N7-C5	20.32	1.51	1.39
2	K	1	A	N7-C5	20.13	1.51	1.39

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	A	C8-N9-C4	44.37	123.55	105.80
2	J	1	A	C8-N9-C4	42.73	122.89	105.80
2	I	1	A	C8-N9-C4	40.98	122.19	105.80
2	K	1	A	C8-N9-C4	39.78	121.71	105.80
2	H	1	A	C8-N9-C4	38.65	121.26	105.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	3518	0	3466	23	0
1	B	3518	0	3466	20	0
1	C	3518	0	3466	15	0
1	D	3489	0	3440	26	0
1	E	3513	0	3461	24	0
1	F	3338	0	3278	20	0
2	G	66	0	33	1	0
2	H	66	0	33	1	0
2	I	66	0	33	0	0
2	J	66	0	33	3	0
2	K	66	0	33	1	0
2	L	66	0	33	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	84	0	0	5	0
4	B	76	0	0	4	0
4	C	90	0	0	0	0
4	D	83	0	0	6	0
4	E	81	0	0	2	0
4	F	71	0	0	0	0
4	H	1	0	0	0	0
4	J	2	0	0	0	0
4	K	3	0	0	0	0
4	L	1	0	0	0	0
All	All	21812	0	20775	127	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 3.

The worst 5 of 127 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:B:199:GLN:OE1	4:B:601:HOH:O	1.84	0.94
1:A:424:ILE:O	4:A:601:HOH:O	1.99	0.80
1:E:75:ALA:HA	1:E:110:ILE:HD11	1.65	0.79
1:E:416:LYS:NZ	4:E:602:HOH:O	2.18	0.77
1:A:263:ARG:NH2	4:A:604:HOH:O	2.21	0.73

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	434/462 (94%)	422 (97%)	12 (3%)	0	100	100
1	B	434/462 (94%)	421 (97%)	13 (3%)	0	100	100
1	C	434/462 (94%)	417 (96%)	16 (4%)	1 (0%)	47	62
1	D	429/462 (93%)	417 (97%)	11 (3%)	1 (0%)	47	62
1	E	433/462 (94%)	417 (96%)	16 (4%)	0	100	100
1	F	403/462 (87%)	389 (96%)	14 (4%)	0	100	100
All	All	2567/2772 (93%)	2483 (97%)	82 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	LYS
1	D	441	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	392/411 (95%)	387 (99%)	5 (1%)	69	84
1	B	392/411 (95%)	387 (99%)	5 (1%)	69	84
1	C	392/411 (95%)	387 (99%)	5 (1%)	69	84
1	D	389/411 (95%)	386 (99%)	3 (1%)	81	91
1	E	392/411 (95%)	387 (99%)	5 (1%)	69	84
1	F	373/411 (91%)	366 (98%)	7 (2%)	57	75
All	All	2330/2466 (94%)	2300 (99%)	30 (1%)	69	84

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	412	LYS
1	D	334	HIS
1	F	324	HIS
1	D	113	LEU
1	D	416	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	231	GLN
1	D	181	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	2/3 (66%)	1 (50%)	1 (50%)
2	H	2/3 (66%)	2 (100%)	1 (50%)
2	I	2/3 (66%)	2 (100%)	0
2	J	2/3 (66%)	2 (100%)	1 (50%)
2	K	2/3 (66%)	2 (100%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L	2/3 (66%)	2 (100%)	0
All	All	12/18 (66%)	11 (91%)	3 (25%)

5 of 11 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	3	A
2	H	2	A
2	H	3	A
2	I	2	A
2	I	3	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	G	2	A
2	H	2	A
2	J	2	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	501	-	4,4,4	0.12	0	6,6,6	0.08	0
3	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	E	501	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.06	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	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<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	438/462 (94%)	0.03	20 (4%) 32 31	37, 55, 102, 135	0
1	B	438/462 (94%)	0.04	19 (4%) 35 33	41, 59, 100, 117	0
1	C	438/462 (94%)	0.14	32 (7%) 15 13	38, 59, 118, 158	0
1	D	435/462 (94%)	0.34	39 (8%) 9 8	37, 62, 133, 170	0
1	E	437/462 (94%)	0.01	13 (2%) 50 49	36, 55, 98, 122	0
1	F	415/462 (89%)	0.39	48 (11%) 4 4	38, 61, 121, 152	0
2	G	3/3 (100%)	-0.34	0 100 100	54, 54, 55, 58	0
2	H	3/3 (100%)	-0.55	0 100 100	58, 58, 60, 62	0
2	I	3/3 (100%)	-0.46	0 100 100	66, 66, 69, 72	0
2	J	3/3 (100%)	-0.09	0 100 100	75, 75, 77, 80	0
2	K	3/3 (100%)	-0.97	0 100 100	56, 56, 59, 60	0
2	L	3/3 (100%)	-0.79	0 100 100	67, 67, 72, 72	0
All	All	2619/2790 (93%)	0.15	171 (6%) 18 17	36, 58, 117, 170	0

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	348	VAL	10.4
1	F	411	PHE	9.3
1	D	347	ALA	7.6
1	B	347	ALA	6.4
1	B	348	VAL	6.4

### 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](#)

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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	501	5/5	0.96	0.12	53,57,58,68	0
3	SO4	C	501	5/5	0.97	0.13	48,56,64,69	0
3	SO4	B	501	5/5	0.97	0.12	60,64,69,69	0
3	SO4	A	501	5/5	0.98	0.10	59,63,66,74	0
3	SO4	F	501	5/5	0.98	0.11	56,62,68,70	0
3	SO4	E	501	5/5	0.99	0.14	58,60,64,65	0

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

There are no such residues in this entry.