



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 12:30 PM BST

PDB ID : 5WHV  
Title : Crystal structure of ArtB  
Authors : Gao, X.; Galan, J.E.  
Deposited on : 2017-07-18  
Resolution : 2.30 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.

---

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

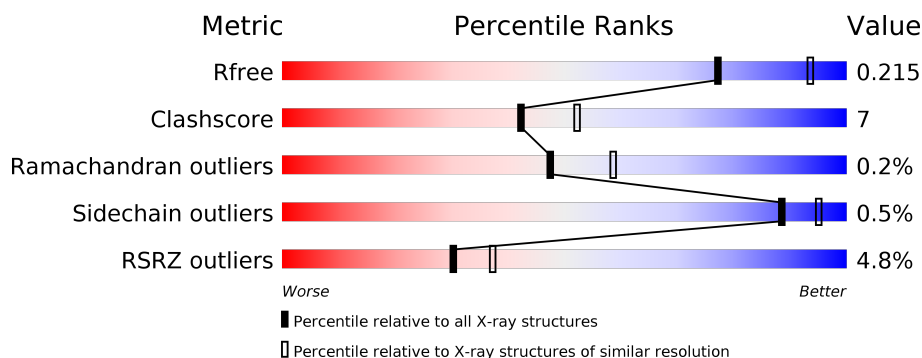
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	149	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>21%</div> </div> </div>
1	B	149	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>12%</div> <div>21%</div> </div> </div>
1	C	149	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>•</div> <div>21%</div> </div> </div>
1	D	149	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>12%</div> <div>21%</div> </div> </div>
1	E	149	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>21%</div> </div> </div>
1	F	149	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>8%</div> <div>20%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	149	
1	H	149	
1	I	149	
1	J	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	A	201	-	-	X	-
2	PEG	B	202	-	-	-	X
2	PEG	D	201	-	-	X	-
2	PEG	E	201	-	-	X	-
2	PEG	H	201	-	-	X	-
2	PEG	H	203	-	-	-	X
2	PEG	I	201	-	-	X	-
4	CL	E	204	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10810 atoms, of which 301 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 ArtB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	1	0
			947	594	160	186	7			
1	B	118	Total	C	N	O	S	0	1	0
			947	594	160	186	7			
1	C	118	Total	C	N	O	S	0	0	0
			939	590	158	184	7			
1	D	118	Total	C	N	O	S	0	0	0
			939	590	158	184	7			
1	E	118	Total	C	N	O	S	0	0	0
			939	590	158	184	7			
1	F	119	Total	C	N	O	S	0	0	0
			944	593	159	185	7			
1	G	119	Total	C	N	O	S	0	0	0
			946	595	159	185	7			
1	H	125	Total	C	N	O	S	0	0	0
			993	624	169	193	7			
1	I	118	Total	C	N	O	S	0	0	0
			939	590	158	184	7			
1	J	128	Total	C	N	O	S	0	1	0
			1039	650	183	199	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	LEU	-	expression tag	UNP Q404H3
A	143	GLU	-	expression tag	UNP Q404H3
A	144	HIS	-	expression tag	UNP Q404H3
A	145	HIS	-	expression tag	UNP Q404H3
A	146	HIS	-	expression tag	UNP Q404H3
A	147	HIS	-	expression tag	UNP Q404H3
A	148	HIS	-	expression tag	UNP Q404H3
A	149	HIS	-	expression tag	UNP Q404H3
B	142	LEU	-	expression tag	UNP Q404H3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	143	GLU	-	expression tag	UNP Q404H3
B	144	HIS	-	expression tag	UNP Q404H3
B	145	HIS	-	expression tag	UNP Q404H3
B	146	HIS	-	expression tag	UNP Q404H3
B	147	HIS	-	expression tag	UNP Q404H3
B	148	HIS	-	expression tag	UNP Q404H3
B	149	HIS	-	expression tag	UNP Q404H3
C	142	LEU	-	expression tag	UNP Q404H3
C	143	GLU	-	expression tag	UNP Q404H3
C	144	HIS	-	expression tag	UNP Q404H3
C	145	HIS	-	expression tag	UNP Q404H3
C	146	HIS	-	expression tag	UNP Q404H3
C	147	HIS	-	expression tag	UNP Q404H3
C	148	HIS	-	expression tag	UNP Q404H3
C	149	HIS	-	expression tag	UNP Q404H3
D	142	LEU	-	expression tag	UNP Q404H3
D	143	GLU	-	expression tag	UNP Q404H3
D	144	HIS	-	expression tag	UNP Q404H3
D	145	HIS	-	expression tag	UNP Q404H3
D	146	HIS	-	expression tag	UNP Q404H3
D	147	HIS	-	expression tag	UNP Q404H3
D	148	HIS	-	expression tag	UNP Q404H3
D	149	HIS	-	expression tag	UNP Q404H3
E	142	LEU	-	expression tag	UNP Q404H3
E	143	GLU	-	expression tag	UNP Q404H3
E	144	HIS	-	expression tag	UNP Q404H3
E	145	HIS	-	expression tag	UNP Q404H3
E	146	HIS	-	expression tag	UNP Q404H3
E	147	HIS	-	expression tag	UNP Q404H3
E	148	HIS	-	expression tag	UNP Q404H3
E	149	HIS	-	expression tag	UNP Q404H3
F	142	LEU	-	expression tag	UNP Q404H3
F	143	GLU	-	expression tag	UNP Q404H3
F	144	HIS	-	expression tag	UNP Q404H3
F	145	HIS	-	expression tag	UNP Q404H3
F	146	HIS	-	expression tag	UNP Q404H3
F	147	HIS	-	expression tag	UNP Q404H3
F	148	HIS	-	expression tag	UNP Q404H3
F	149	HIS	-	expression tag	UNP Q404H3
G	142	LEU	-	expression tag	UNP Q404H3
G	143	GLU	-	expression tag	UNP Q404H3
G	144	HIS	-	expression tag	UNP Q404H3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	145	HIS	-	expression tag	UNP Q404H3
G	146	HIS	-	expression tag	UNP Q404H3
G	147	HIS	-	expression tag	UNP Q404H3
G	148	HIS	-	expression tag	UNP Q404H3
G	149	HIS	-	expression tag	UNP Q404H3
H	142	LEU	-	expression tag	UNP Q404H3
H	143	GLU	-	expression tag	UNP Q404H3
H	144	HIS	-	expression tag	UNP Q404H3
H	145	HIS	-	expression tag	UNP Q404H3
H	146	HIS	-	expression tag	UNP Q404H3
H	147	HIS	-	expression tag	UNP Q404H3
H	148	HIS	-	expression tag	UNP Q404H3
H	149	HIS	-	expression tag	UNP Q404H3
I	142	LEU	-	expression tag	UNP Q404H3
I	143	GLU	-	expression tag	UNP Q404H3
I	144	HIS	-	expression tag	UNP Q404H3
I	145	HIS	-	expression tag	UNP Q404H3
I	146	HIS	-	expression tag	UNP Q404H3
I	147	HIS	-	expression tag	UNP Q404H3
I	148	HIS	-	expression tag	UNP Q404H3
I	149	HIS	-	expression tag	UNP Q404H3
J	142	LEU	-	expression tag	UNP Q404H3
J	143	GLU	-	expression tag	UNP Q404H3
J	144	HIS	-	expression tag	UNP Q404H3
J	145	HIS	-	expression tag	UNP Q404H3
J	146	HIS	-	expression tag	UNP Q404H3
J	147	HIS	-	expression tag	UNP Q404H3
J	148	HIS	-	expression tag	UNP Q404H3
J	149	HIS	-	expression tag	UNP Q404H3

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



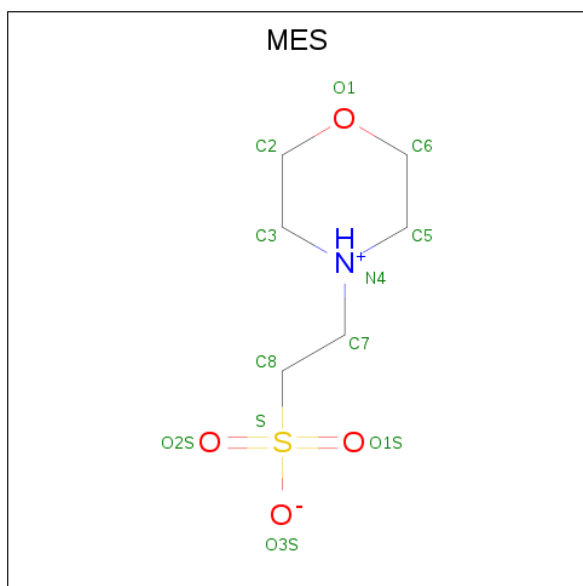
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		
2	E	1	Total	C	H	O	0	0
			17	4	10	3		
2	E	1	Total	C	H	O	0	0
			17	4	10	3		
2	E	1	Total	C	H	O	0	0
			17	4	10	3		
2	F	1	Total	C	H	O	0	0
			17	4	10	3		
2	F	1	Total	C	H	O	0	0
			17	4	10	3		
2	F	1	Total	C	H	O	0	0
			17	4	10	3		
2	F	1	Total	C	H	O	0	0
			17	4	10	3		
2	G	1	Total	C	H	O	0	0
			17	4	10	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	H	O	0	0
			17	4	10	3		
2	H	1	Total	C	H	O	0	0
			17	4	10	3		
2	H	1	Total	C	H	O	0	0
			17	4	10	3		
2	H	1	Total	C	H	O	0	0
			17	4	10	3		
2	I	1	Total	C	H	O	0	0
			17	4	10	3		
2	I	1	Total	C	H	O	0	0
			17	4	10	3		
2	J	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
3	B	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
3	C	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
3	G	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
3	I	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	
3	J	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Cl	0	0
			1	1		
4	J	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		
4	I	2	Total	Cl	0	0
			2	2		
4	C	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Ca	0	0
			1	1		
5	J	1	Total	Ca	0	0
			1	1		
5	E	2	Total	Ca	0	0
			2	2		
5	H	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	Ca 1	0	0
5	A	1	Total 1	Ca 1	0	0
5	F	1	Total 1	Ca 1	0	0

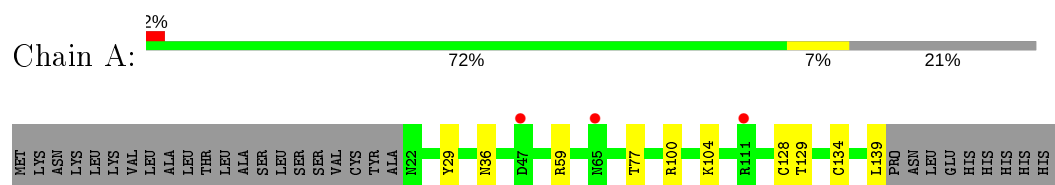
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	60	Total 60	O 60	0	0
6	B	52	Total 52	O 52	0	0
6	C	51	Total 51	O 51	0	0
6	D	56	Total 56	O 56	0	0
6	E	58	Total 58	O 58	0	0
6	F	87	Total 87	O 87	0	0
6	G	59	Total 59	O 59	0	0
6	H	94	Total 94	O 94	0	0
6	I	78	Total 78	O 78	0	0
6	J	91	Total 91	O 91	0	0

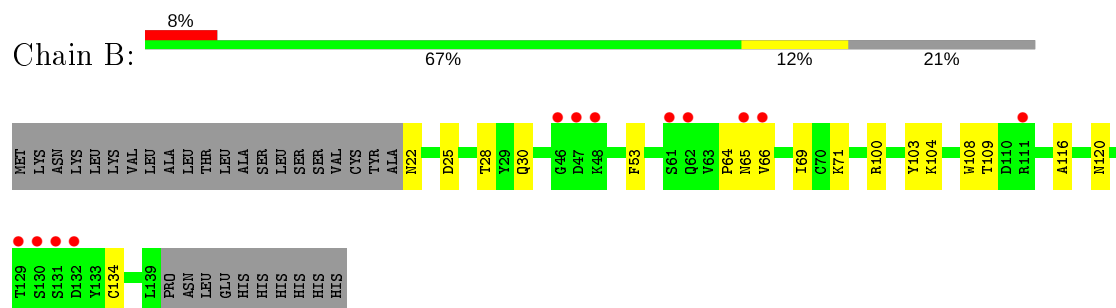
### 3 Residue-property plots [i](#)

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.

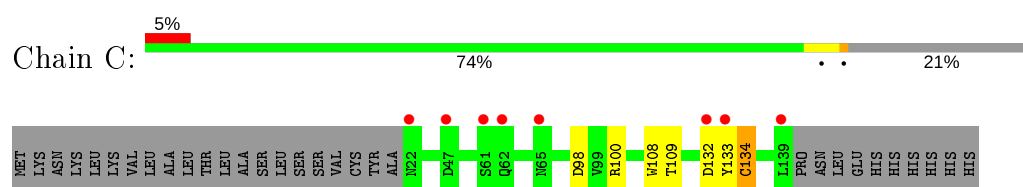
- Molecule 1: ArtB protein



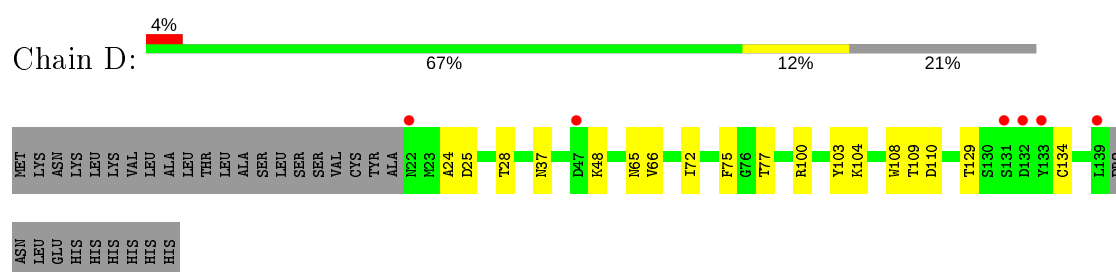
- Molecule 1: ArtB protein



- Molecule 1: ArtB protein



- Molecule 1: ArtB protein

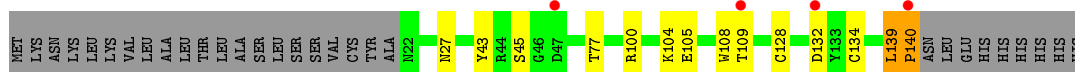


- Molecule 1: ArtB protein

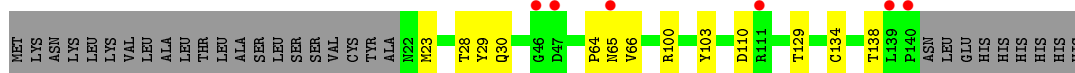




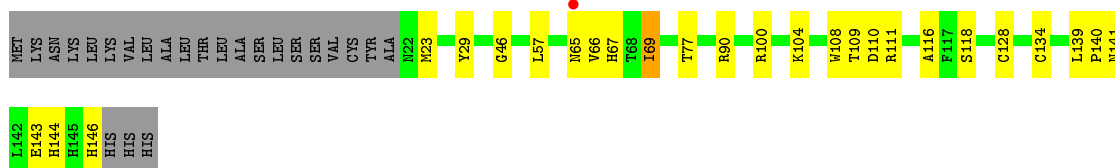
- Molecule 1: ArtB protein



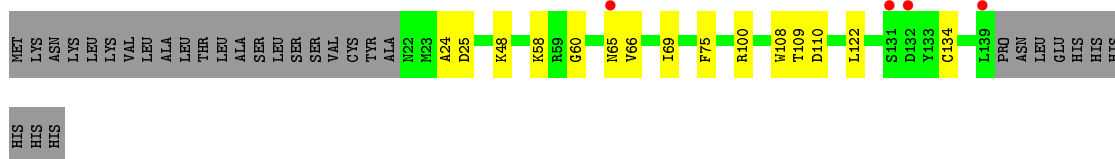
- Molecule 1: ArtB protein



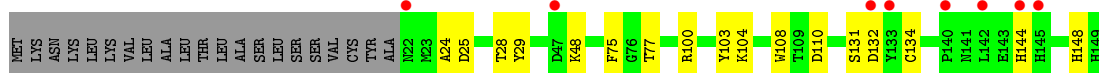
- Molecule 1: ArtB protein



- Molecule 1: ArtB protein



- Molecule 1: ArtB protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.87Å 94.23Å 125.23Å 90.00° 103.62° 90.00°	Depositor
Resolution (Å)	31.12 – 2.30 31.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (31.12-2.30) 96.6 (31.12-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.72 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.167 , 0.213 0.170 , 0.215	Depositor DCC
$R_{free}$ test set	3418 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PEG, MES, CL

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	0.45	0/968	0.58	0/1312
1	B	0.44	0/968	0.56	0/1312
1	C	0.45	0/960	0.66	2/1301 (0.2%)
1	D	0.44	0/960	0.58	0/1301
1	E	0.43	0/960	0.55	0/1301
1	F	0.45	0/965	0.62	1/1308 (0.1%)
1	G	0.42	0/968	0.58	0/1313
1	H	0.45	0/1017	0.59	0/1380
1	I	0.44	0/960	0.60	0/1301
1	J	0.42	0/1067	0.56	0/1448
All	All	0.44	0/9793	0.59	3/13277 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	TYR	C-N-CA	8.22	142.26	121.70
1	F	140	PRO	N-CA-CB	6.55	111.16	103.30
1	C	132	ASP	N-CA-C	5.18	124.97	111.00

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	947	0	883	9	0
1	B	947	0	883	21	0
1	C	939	0	878	5	0
1	D	939	0	878	12	0
1	E	939	0	878	10	0
1	F	944	0	879	11	0
1	G	946	0	885	8	0
1	H	993	0	920	31	0
1	I	939	0	878	14	0
1	J	1039	0	955	10	0
2	A	7	10	10	6	0
2	B	14	20	20	5	0
2	C	7	10	10	3	0
2	D	7	10	10	4	0
2	E	21	30	30	6	0
2	F	35	50	50	5	0
2	G	14	20	20	3	0
2	H	21	30	30	8	0
2	I	14	20	20	7	0
2	J	7	10	10	2	0
3	A	12	13	12	3	0
3	B	12	13	13	2	0
3	C	12	13	13	0	0
3	G	12	13	13	1	0
3	H	12	13	13	1	0
3	I	12	13	13	0	0
3	J	12	13	13	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	2	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	I	2	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	1	0	0	0	0
6	A	60	0	0	0	0
6	B	52	0	0	1	0
6	C	51	0	0	0	0
6	D	56	0	0	0	0
6	E	58	0	0	1	0
6	F	87	0	0	2	0
6	G	59	0	0	0	0
6	H	94	0	0	5	0
6	I	78	0	0	1	0
6	J	91	0	0	0	0
All	All	10509	301	9217	131	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.

The worst 5 of 131 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:30:GLN:NE2	1:B:65:ASN:OD1	1.86	1.07
1:H:109:THR:H	2:H:201:PEG:H42	1.28	0.97
1:H:65:ASN:OD1	1:H:66:VAL:N	1.97	0.96
1:F:109:THR:H	2:F:204:PEG:H22	1.33	0.93
1:H:111:ARG:NH2	6:H:301:HOH:O	2.01	0.91

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	117/149 (78%)	114 (97%)	3 (3%)	0	<b>100</b> <b>100</b>

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	117/149 (78%)	113 (97%)	4 (3%)	0	100	100
1	C	116/149 (78%)	110 (95%)	5 (4%)	1 (1%)	17	20
1	D	116/149 (78%)	114 (98%)	2 (2%)	0	100	100
1	E	116/149 (78%)	113 (97%)	3 (3%)	0	100	100
1	F	117/149 (78%)	113 (97%)	3 (3%)	1 (1%)	17	20
1	G	117/149 (78%)	114 (97%)	3 (3%)	0	100	100
1	H	123/149 (83%)	121 (98%)	2 (2%)	0	100	100
1	I	116/149 (78%)	115 (99%)	1 (1%)	0	100	100
1	J	127/149 (85%)	125 (98%)	2 (2%)	0	100	100
All	All	1182/1490 (79%)	1152 (98%)	28 (2%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	134	CYS
1	F	139	LEU

### 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	103/130 (79%)	103 (100%)	0	100	100
1	B	103/130 (79%)	103 (100%)	0	100	100
1	C	102/130 (78%)	102 (100%)	0	100	100
1	D	102/130 (78%)	101 (99%)	1 (1%)	76	87
1	E	102/130 (78%)	102 (100%)	0	100	100
1	F	102/130 (78%)	101 (99%)	1 (1%)	76	87
1	G	103/130 (79%)	102 (99%)	1 (1%)	76	87
1	H	107/130 (82%)	105 (98%)	2 (2%)	57	73
1	I	102/130 (78%)	102 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	113/130 (87%)	113 (100%)	0	100	100
All	All	1039/1300 (80%)	1034 (100%)	5 (0%)	88	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	129	THR
1	F	132	ASP
1	G	129	THR
1	H	57	LEU
1	H	69	ILE

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	30	GLN
1	H	141	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 48 ligands modelled in this entry, 20 are monoatomic - leaving 28 for Mogul analysis.

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	MES	J	202	-	12,12,12	2.07	1 (8%)	14,16,16	1.63	4 (28%)
2	PEG	E	203	-	6,6,6	0.55	0	5,5,5	0.28	0
2	PEG	H	203	-	6,6,6	0.56	0	5,5,5	0.62	0
2	PEG	I	201	-	6,6,6	0.51	0	5,5,5	0.34	0
3	MES	C	202	-	12,12,12	2.05	1 (8%)	14,16,16	1.76	3 (21%)
2	PEG	E	202	-	6,6,6	0.49	0	5,5,5	0.36	0
3	MES	A	202	-	12,12,12	2.16	1 (8%)	14,16,16	1.64	5 (35%)
2	PEG	F	201	-	6,6,6	0.42	0	5,5,5	0.45	0
2	PEG	E	201	-	6,6,6	0.54	0	5,5,5	0.55	0
2	PEG	H	202	-	6,6,6	0.57	0	5,5,5	0.39	0
2	PEG	G	201	-	6,6,6	0.55	0	5,5,5	0.60	0
2	PEG	G	202	-	6,6,6	0.54	0	5,5,5	0.38	0
3	MES	G	203	-	12,12,12	2.15	1 (8%)	14,16,16	1.66	4 (28%)
2	PEG	B	202	-	6,6,6	0.55	0	5,5,5	0.22	0
2	PEG	B	201	-	6,6,6	0.50	0	5,5,5	0.17	0
2	PEG	D	201	-	6,6,6	0.47	0	5,5,5	0.68	0
2	PEG	F	204	-	6,6,6	0.53	0	5,5,5	0.41	0
2	PEG	C	201	-	6,6,6	0.49	0	5,5,5	0.69	0
2	PEG	I	202	-	6,6,6	0.45	0	5,5,5	0.72	0
3	MES	I	203	-	12,12,12	2.10	1 (8%)	14,16,16	1.61	4 (28%)
2	PEG	F	205	-	6,6,6	0.53	0	5,5,5	0.47	0
3	MES	B	203	-	12,12,12	1.92	1 (8%)	14,16,16	1.99	4 (28%)
2	PEG	F	202	-	6,6,6	0.73	0	5,5,5	1.00	0
2	PEG	F	203	-	6,6,6	0.49	0	5,5,5	0.22	0
2	PEG	A	201	-	6,6,6	0.51	0	5,5,5	0.37	0
2	PEG	H	201	-	6,6,6	0.58	0	5,5,5	0.56	0
2	PEG	J	201	-	6,6,6	0.43	0	5,5,5	0.60	0
3	MES	H	204	-	12,12,12	2.16	1 (8%)	14,16,16	1.62	4 (28%)

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
3	MES	J	202	-	-	4/6/14/14	0/1/1/1
2	PEG	E	203	-	-	2/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	H	203	-	-	0/4/4/4	-
2	PEG	I	201	-	-	2/4/4/4	-
3	MES	C	202	-	-	5/6/14/14	0/1/1/1
2	PEG	E	202	-	-	3/4/4/4	-
3	MES	A	202	-	-	3/6/14/14	0/1/1/1
2	PEG	F	201	-	-	3/4/4/4	-
2	PEG	E	201	-	-	2/4/4/4	-
2	PEG	H	202	-	-	2/4/4/4	-
2	PEG	G	201	-	-	1/4/4/4	-
2	PEG	G	202	-	-	3/4/4/4	-
3	MES	G	203	-	-	1/6/14/14	0/1/1/1
2	PEG	B	202	-	-	1/4/4/4	-
2	PEG	B	201	-	-	4/4/4/4	-
2	PEG	D	201	-	-	2/4/4/4	-
2	PEG	F	204	-	-	2/4/4/4	-
2	PEG	C	201	-	-	3/4/4/4	-
2	PEG	I	202	-	-	1/4/4/4	-
3	MES	I	203	-	-	3/6/14/14	0/1/1/1
2	PEG	F	205	-	-	2/4/4/4	-
3	MES	B	203	-	-	2/6/14/14	0/1/1/1
2	PEG	F	202	-	-	2/4/4/4	-
2	PEG	F	203	-	-	3/4/4/4	-
2	PEG	A	201	-	-	0/4/4/4	-
2	PEG	H	201	-	-	2/4/4/4	-
2	PEG	J	201	-	-	2/4/4/4	-
3	MES	H	204	-	-	5/6/14/14	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	MES	C8-S	-7.16	1.67	1.77
3	H	204	MES	C8-S	-7.14	1.67	1.77
3	G	203	MES	C8-S	-7.07	1.67	1.77
3	I	203	MES	C8-S	-6.93	1.67	1.77
3	J	202	MES	C8-S	-6.83	1.67	1.77

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	203	MES	C5-N4-C3	4.30	118.50	108.83
3	C	202	MES	C5-N4-C3	3.73	117.23	108.83
3	B	203	MES	O3S-S-C8	3.28	111.07	105.77
3	C	202	MES	O3S-S-C8	3.27	111.06	105.77
3	B	203	MES	O2S-S-C8	3.19	110.76	106.92

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	202	MES	N4-C7-C8-S
3	J	202	MES	C7-C8-S-O1S
3	C	202	MES	N4-C7-C8-S
3	A	202	MES	C8-C7-N4-C3
3	A	202	MES	C8-C7-N4-C5

There are no ring outliers.

22 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	202	MES	1	0
2	E	203	PEG	1	0
2	H	203	PEG	2	0
2	I	201	PEG	7	0
3	A	202	MES	3	0
2	F	201	PEG	1	0
2	E	201	PEG	5	0
2	H	202	PEG	2	0
2	G	201	PEG	1	0
2	G	202	PEG	2	0
3	G	203	MES	1	0
2	B	202	PEG	2	0
2	B	201	PEG	3	0
2	D	201	PEG	4	0
2	F	204	PEG	3	0
2	C	201	PEG	3	0
3	B	203	MES	2	0
2	F	202	PEG	1	0
2	A	201	PEG	6	0
2	H	201	PEG	4	0
2	J	201	PEG	2	0
3	H	204	MES	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	118/149 (79%)	-0.21	3 (2%) 57 64	17, 29, 53, 70	0
1	B	118/149 (79%)	0.14	12 (10%) 6 9	19, 33, 70, 99	0
1	C	118/149 (79%)	-0.01	8 (6%) 17 22	20, 30, 60, 84	0
1	D	118/149 (79%)	-0.07	6 (5%) 28 35	20, 30, 56, 95	0
1	E	118/149 (79%)	0.01	5 (4%) 36 43	18, 33, 62, 92	0
1	F	119/149 (79%)	-0.26	4 (3%) 45 52	14, 23, 56, 72	0
1	G	119/149 (79%)	-0.16	6 (5%) 28 35	15, 26, 62, 82	0
1	H	125/149 (83%)	-0.11	1 (0%) 86 89	14, 23, 52, 82	0
1	I	118/149 (79%)	-0.21	4 (3%) 45 52	14, 25, 51, 80	0
1	J	128/149 (85%)	0.08	8 (6%) 20 25	15, 25, 53, 80	0
All	All	1199/1490 (80%)	-0.08	57 (4%) 30 37	14, 27, 58, 99	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	TYR	6.5
1	E	132	ASP	6.1
1	B	65	ASN	6.1
1	B	131	SER	5.7
1	J	142	LEU	5.1

### 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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
2	PEG	H	203	7/7	0.53	0.42	62,76,92,92	0
2	PEG	F	205	7/7	0.59	0.27	68,82,88,91	0
2	PEG	F	204	7/7	0.68	0.31	61,74,77,77	0
2	PEG	G	202	7/7	0.68	0.32	58,72,87,89	0
2	PEG	B	202	7/7	0.74	0.54	73,88,105,106	0
2	PEG	E	202	7/7	0.75	0.29	68,81,93,93	0
2	PEG	I	202	7/7	0.75	0.36	50,60,69,71	0
2	PEG	E	201	7/7	0.75	0.25	51,62,72,74	0
2	PEG	A	201	7/7	0.79	0.27	49,59,71,71	0
2	PEG	H	202	7/7	0.80	0.27	34,52,66,66	0
2	PEG	F	202	7/7	0.81	0.17	27,33,44,46	0
2	PEG	B	201	7/7	0.82	0.22	57,68,73,75	0
2	PEG	E	203	7/7	0.83	0.36	35,49,73,79	0
3	MES	B	203	12/12	0.83	0.32	50,64,85,86	0
3	MES	G	203	12/12	0.83	0.30	55,74,96,98	0
2	PEG	G	201	7/7	0.83	0.19	44,53,60,61	0
3	MES	C	202	12/12	0.84	0.31	65,79,93,96	0
2	PEG	F	201	7/7	0.85	0.20	43,57,80,81	0
3	MES	A	202	12/12	0.85	0.31	63,78,93,95	0
2	PEG	F	203	7/7	0.86	0.16	48,61,76,79	0
4	CL	E	204	1/1	0.87	0.17	71,71,71,71	0
4	CL	I	204	1/1	0.88	0.15	63,63,63,63	0
3	MES	J	202	12/12	0.88	0.24	43,59,117,118	0
3	MES	I	203	12/12	0.88	0.25	39,56,95,98	0
2	PEG	C	201	7/7	0.88	0.16	27,44,55,58	0
5	CA	B	205	1/1	0.91	0.11	64,64,64,64	0
4	CL	C	203	1/1	0.92	0.12	56,56,56,56	0
4	CL	B	204	1/1	0.92	0.12	63,63,63,63	0
3	MES	H	204	12/12	0.92	0.17	36,48,71,75	0
2	PEG	I	201	7/7	0.93	0.11	21,38,53,54	0
4	CL	G	204	1/1	0.93	0.09	60,60,60,60	0
2	PEG	J	201	7/7	0.93	0.19	34,46,56,56	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	D	201	7/7	0.93	0.15	31,39,47,53	0
4	CL	E	205	1/1	0.94	0.10	50,50,50,50	0
2	PEG	H	201	7/7	0.96	0.13	30,37,48,52	0
4	CL	D	202	1/1	0.96	0.14	56,56,56,56	0
4	CL	A	203	1/1	0.96	0.12	50,50,50,50	0
4	CL	F	206	1/1	0.97	0.08	42,42,42,42	0
4	CL	I	205	1/1	0.97	0.10	48,48,48,48	0
5	CA	E	207	1/1	0.98	0.11	54,54,54,54	0
5	CA	J	204	1/1	0.98	0.07	44,44,44,44	0
5	CA	F	207	1/1	0.98	0.04	38,38,38,38	0
5	CA	I	206	1/1	0.98	0.04	43,43,43,43	0
5	CA	E	206	1/1	0.98	0.05	49,49,49,49	0
5	CA	A	204	1/1	0.99	0.03	21,21,21,21	0
4	CL	J	203	1/1	0.99	0.15	42,42,42,42	0
5	CA	G	205	1/1	0.99	0.07	43,43,43,43	0
5	CA	H	205	1/1	0.99	0.09	25,25,25,25	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.