



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:40 am BST

PDB ID : 6OJY  
Title : Methylated PilT4 from *Geobacter metallireducens* bound to sulfate: C3ocococ conformation  
Authors : McCallum, M.; Howell, P.L.  
Deposited on : 2019-04-12  
Resolution : 3.30 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	:	2.11
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)	:	2.11

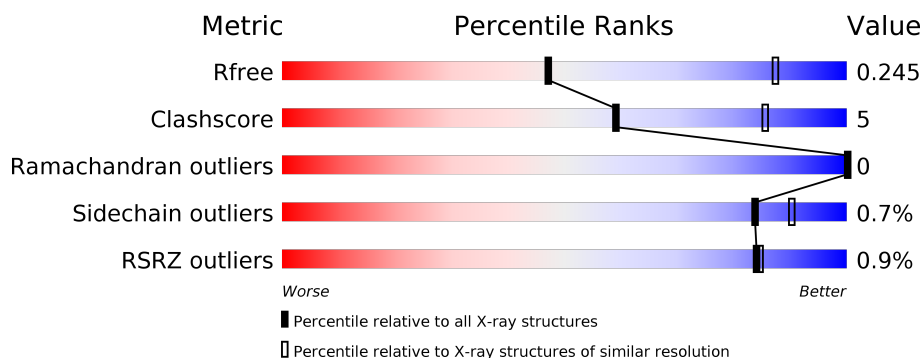
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	385	<div> <div>83%</div> <div>8%</div> <div>8%</div> </div>
2	B	385	<div> <div>2%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
3	C	385	<div> <div>2%</div> <div>82%</div> <div>10%</div> <div>8%</div> </div>
4	D	385	<div> <div>78%</div> <div>12%</div> <div>9%</div> </div>
4	E	385	<div> <div>80%</div> <div>12%</div> <div>8%</div> </div>
5	F	385	<div> <div>2%</div> <div>80%</div> <div>11%</div> <div>9%</div> </div>

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
6	SO4	B	401	-	-	X	-
6	SO4	D	401	-	-	X	-
6	SO4	E	401	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16453 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 Twitching motility pilus retraction ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2726	1726	476	510	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q39VU6
A	-18	GLY	-	expression tag	UNP Q39VU6
A	-17	SER	-	expression tag	UNP Q39VU6
A	-16	SER	-	expression tag	UNP Q39VU6
A	-15	HIS	-	expression tag	UNP Q39VU6
A	-14	HIS	-	expression tag	UNP Q39VU6
A	-13	HIS	-	expression tag	UNP Q39VU6
A	-12	HIS	-	expression tag	UNP Q39VU6
A	-11	HIS	-	expression tag	UNP Q39VU6
A	-10	HIS	-	expression tag	UNP Q39VU6
A	-9	SER	-	expression tag	UNP Q39VU6
A	-8	SER	-	expression tag	UNP Q39VU6
A	-7	GLY	-	expression tag	UNP Q39VU6
A	-6	LEU	-	expression tag	UNP Q39VU6
A	-5	VAL	-	expression tag	UNP Q39VU6
A	-4	PRO	-	expression tag	UNP Q39VU6
A	-3	ARG	-	expression tag	UNP Q39VU6
A	-2	GLY	-	expression tag	UNP Q39VU6
A	-1	SER	-	expression tag	UNP Q39VU6
A	0	HIS	-	expression tag	UNP Q39VU6

- Molecule 2 is a protein called Twitching motility pilus retraction ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	355	Total	C	N	O	S	0	0	0
			2637	1670	459	494	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q39VU6
B	-18	GLY	-	expression tag	UNP Q39VU6
B	-17	SER	-	expression tag	UNP Q39VU6
B	-16	SER	-	expression tag	UNP Q39VU6
B	-15	HIS	-	expression tag	UNP Q39VU6
B	-14	HIS	-	expression tag	UNP Q39VU6
B	-13	HIS	-	expression tag	UNP Q39VU6
B	-12	HIS	-	expression tag	UNP Q39VU6
B	-11	HIS	-	expression tag	UNP Q39VU6
B	-10	HIS	-	expression tag	UNP Q39VU6
B	-9	SER	-	expression tag	UNP Q39VU6
B	-8	SER	-	expression tag	UNP Q39VU6
B	-7	GLY	-	expression tag	UNP Q39VU6
B	-6	LEU	-	expression tag	UNP Q39VU6
B	-5	VAL	-	expression tag	UNP Q39VU6
B	-4	PRO	-	expression tag	UNP Q39VU6
B	-3	ARG	-	expression tag	UNP Q39VU6
B	-2	GLY	-	expression tag	UNP Q39VU6
B	-1	SER	-	expression tag	UNP Q39VU6
B	0	HIS	-	expression tag	UNP Q39VU6

- Molecule 3 is a protein called Twitching motility pilus retraction ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	355	Total	C	N	O	S	0	0	0
			2713	1715	477	506	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP Q39VU6
C	-18	GLY	-	expression tag	UNP Q39VU6
C	-17	SER	-	expression tag	UNP Q39VU6
C	-16	SER	-	expression tag	UNP Q39VU6
C	-15	HIS	-	expression tag	UNP Q39VU6
C	-14	HIS	-	expression tag	UNP Q39VU6
C	-13	HIS	-	expression tag	UNP Q39VU6
C	-12	HIS	-	expression tag	UNP Q39VU6
C	-11	HIS	-	expression tag	UNP Q39VU6
C	-10	HIS	-	expression tag	UNP Q39VU6
C	-9	SER	-	expression tag	UNP Q39VU6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP Q39VU6
C	-7	GLY	-	expression tag	UNP Q39VU6
C	-6	LEU	-	expression tag	UNP Q39VU6
C	-5	VAL	-	expression tag	UNP Q39VU6
C	-4	PRO	-	expression tag	UNP Q39VU6
C	-3	ARG	-	expression tag	UNP Q39VU6
C	-2	GLY	-	expression tag	UNP Q39VU6
C	-1	SER	-	expression tag	UNP Q39VU6
C	0	HIS	-	expression tag	UNP Q39VU6

- Molecule 4 is a protein called Twitching motility pilus retraction ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	352	Total	C	N	O	S	0	2	0
			2716	1719	481	502	14			
4	E	356	Total	C	N	O	S	0	1	0
			2752	1738	486	514	14			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP Q39VU6
D	-18	GLY	-	expression tag	UNP Q39VU6
D	-17	SER	-	expression tag	UNP Q39VU6
D	-16	SER	-	expression tag	UNP Q39VU6
D	-15	HIS	-	expression tag	UNP Q39VU6
D	-14	HIS	-	expression tag	UNP Q39VU6
D	-13	HIS	-	expression tag	UNP Q39VU6
D	-12	HIS	-	expression tag	UNP Q39VU6
D	-11	HIS	-	expression tag	UNP Q39VU6
D	-10	HIS	-	expression tag	UNP Q39VU6
D	-9	SER	-	expression tag	UNP Q39VU6
D	-8	SER	-	expression tag	UNP Q39VU6
D	-7	GLY	-	expression tag	UNP Q39VU6
D	-6	LEU	-	expression tag	UNP Q39VU6
D	-5	VAL	-	expression tag	UNP Q39VU6
D	-4	PRO	-	expression tag	UNP Q39VU6
D	-3	ARG	-	expression tag	UNP Q39VU6
D	-2	GLY	-	expression tag	UNP Q39VU6
D	-1	SER	-	expression tag	UNP Q39VU6
D	0	HIS	-	expression tag	UNP Q39VU6
E	-19	MET	-	expression tag	UNP Q39VU6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	GLY	-	expression tag	UNP Q39VU6
E	-17	SER	-	expression tag	UNP Q39VU6
E	-16	SER	-	expression tag	UNP Q39VU6
E	-15	HIS	-	expression tag	UNP Q39VU6
E	-14	HIS	-	expression tag	UNP Q39VU6
E	-13	HIS	-	expression tag	UNP Q39VU6
E	-12	HIS	-	expression tag	UNP Q39VU6
E	-11	HIS	-	expression tag	UNP Q39VU6
E	-10	HIS	-	expression tag	UNP Q39VU6
E	-9	SER	-	expression tag	UNP Q39VU6
E	-8	SER	-	expression tag	UNP Q39VU6
E	-7	GLY	-	expression tag	UNP Q39VU6
E	-6	LEU	-	expression tag	UNP Q39VU6
E	-5	VAL	-	expression tag	UNP Q39VU6
E	-4	PRO	-	expression tag	UNP Q39VU6
E	-3	ARG	-	expression tag	UNP Q39VU6
E	-2	GLY	-	expression tag	UNP Q39VU6
E	-1	SER	-	expression tag	UNP Q39VU6
E	0	HIS	-	expression tag	UNP Q39VU6

- Molecule 5 is a protein called Twitching motility pilus retraction ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	352	Total	C	N	O	S	0	1	0
			2688	1708	470	496	14			

There are 20 discrepancies between the modelled and reference sequences:

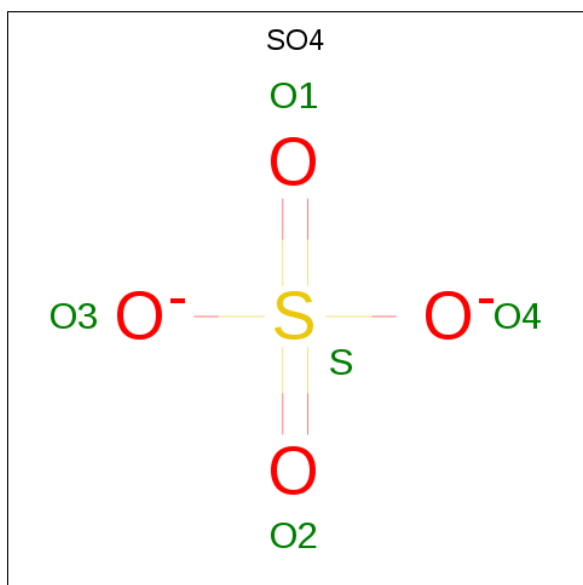
Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q39VU6
F	-18	GLY	-	expression tag	UNP Q39VU6
F	-17	SER	-	expression tag	UNP Q39VU6
F	-16	SER	-	expression tag	UNP Q39VU6
F	-15	HIS	-	expression tag	UNP Q39VU6
F	-14	HIS	-	expression tag	UNP Q39VU6
F	-13	HIS	-	expression tag	UNP Q39VU6
F	-12	HIS	-	expression tag	UNP Q39VU6
F	-11	HIS	-	expression tag	UNP Q39VU6
F	-10	HIS	-	expression tag	UNP Q39VU6
F	-9	SER	-	expression tag	UNP Q39VU6
F	-8	SER	-	expression tag	UNP Q39VU6
F	-7	GLY	-	expression tag	UNP Q39VU6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	LEU	-	expression tag	UNP Q39VU6
F	-5	VAL	-	expression tag	UNP Q39VU6
F	-4	PRO	-	expression tag	UNP Q39VU6
F	-3	ARG	-	expression tag	UNP Q39VU6
F	-2	GLY	-	expression tag	UNP Q39VU6
F	-1	SER	-	expression tag	UNP Q39VU6
F	0	HIS	-	expression tag	UNP Q39VU6

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is water.

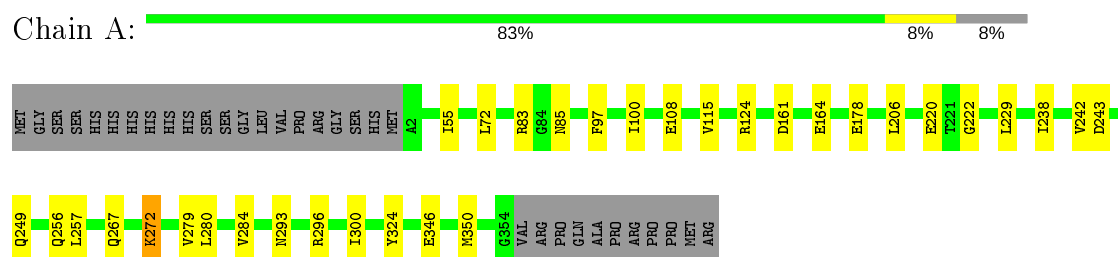


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	43	Total 43	O 43	0	0
7	B	29	Total 29	O 29	0	0
7	C	28	Total 28	O 28	0	0
7	D	35	Total 35	O 35	0	0
7	E	33	Total 33	O 33	0	0
7	F	23	Total 23	O 23	0	0

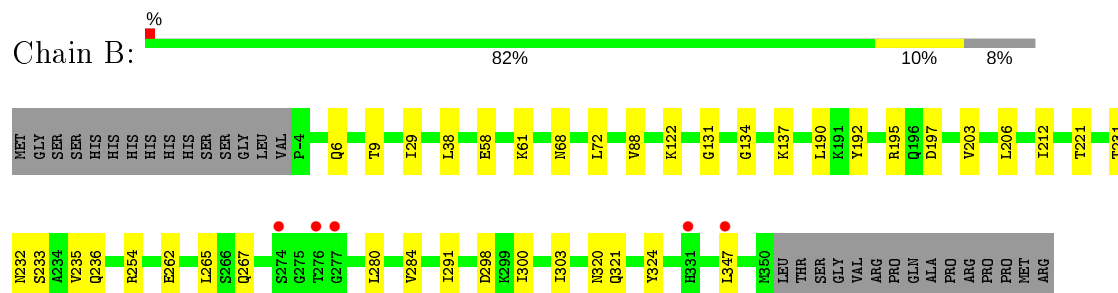
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

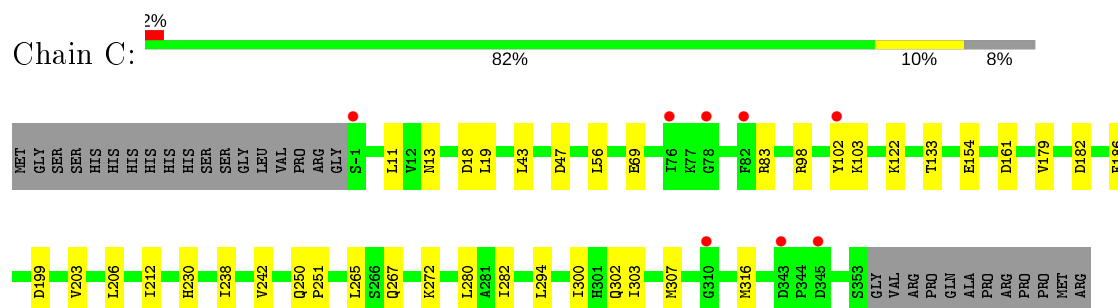
- Molecule 1: Twitching motility pilus retraction ATPase



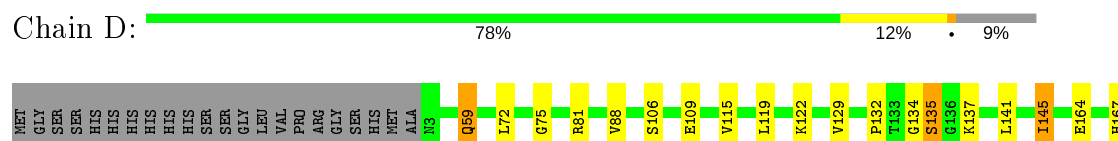
- Molecule 2: Twitching motility pilus retraction ATPase

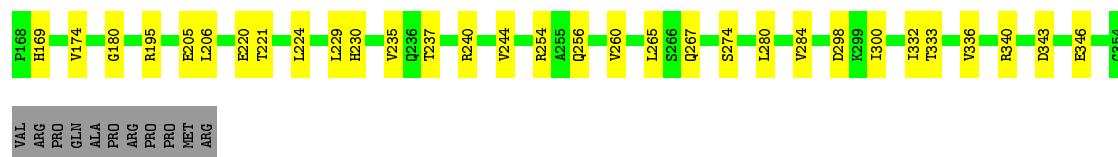


- Molecule 3: Twitching motility pilus retraction ATPase



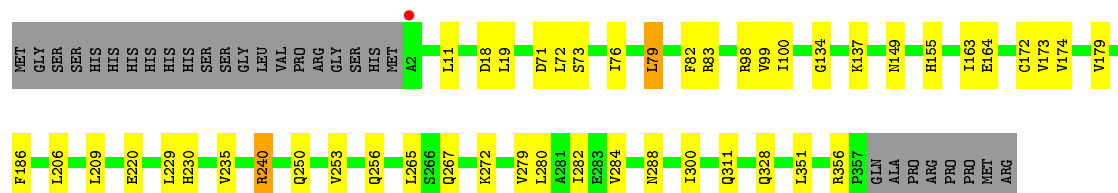
- Molecule 4: Twitching motility pilus retraction ATPase





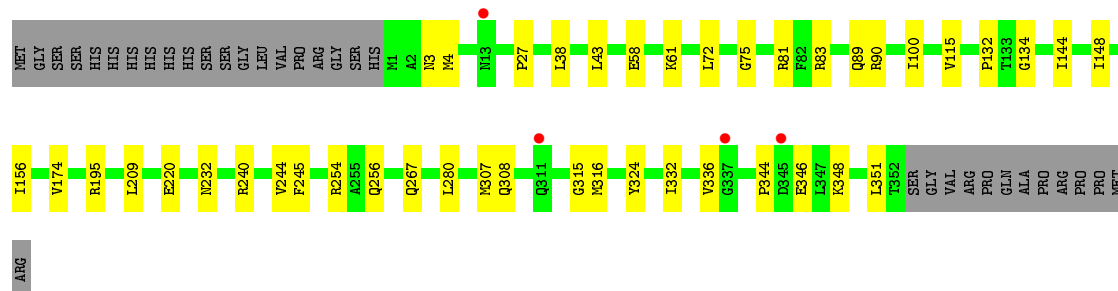
- Molecule 4: Twitching motility pilus retraction ATPase

Chain E: 80% 12% 8%



- Molecule 5: Twitching motility pilus retraction ATPase

Chain F: 80% 11% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.80Å 119.01Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 3.30 48.56 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.56-3.30) 86.2 (48.56-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, $R_{free}$	0.209 , 0.246 0.208 , 0.245	Depositor DCC
$R_{free}$ test set	2274 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.0	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: MLY, 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	0.32	0/2752	0.56	0/3737
2	B	0.32	0/2663	0.55	0/3632
3	C	0.31	0/2739	0.54	0/3724
4	D	0.32	0/2746	0.56	0/3733
4	E	0.32	0/2781	0.55	0/3777
5	F	0.31	0/2725	0.55	0/3705
All	All	0.32	0/16406	0.55	0/22308

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
1	A	0	1
3	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	MLY	Mainchain
3	C	122	MLY	Mainchain

## 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	2726	0	2750	21	0
2	B	2637	0	2578	28	0
3	C	2713	0	2720	30	0
4	D	2716	0	2727	33	0
4	E	2752	0	2776	27	0
5	F	2688	0	2694	27	0
6	A	5	0	0	0	0
6	B	5	0	0	2	0
6	C	5	0	0	0	0
6	D	5	0	0	3	0
6	E	5	0	0	2	0
6	F	5	0	0	1	0
7	A	43	0	0	0	0
7	B	29	0	0	2	0
7	C	28	0	0	5	0
7	D	35	0	0	2	0
7	E	33	0	0	1	0
7	F	23	0	0	1	0
All	All	16453	0	16245	154	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 5.

All (154) 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)
4:D:195[A]:ARG:NH2	4:E:71:ASP:OD2	1.98	0.96
4:D:254:ARG:NH1	7:D:501:HOH:O	2.09	0.83
2:B:321:GLN:HA	2:B:324:TYR:HD1	1.50	0.77
4:D:137:LYS:N	6:D:401:SO4:O4	2.16	0.76
1:A:124:ARG:HD3	1:A:222:GLY:HA2	1.69	0.73
1:A:272:MLY:HG3	1:A:279:VAL:HG13	1.71	0.72
1:A:293:ASN:OD1	1:A:296:ARG:NH2	2.23	0.72
3:C:13:ASN:OD1	7:C:501:HOH:O	2.11	0.68
5:F:83:ARG:HB2	5:F:100:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:NH2	1:A:178:GLU:OE2	2.30	0.65
4:E:267:GLN:HB3	4:E:280:LEU:HD11	1.78	0.64
2:B:267:GLN:HB3	2:B:280:LEU:HD11	1.81	0.63
4:D:340:ARG:HG3	4:D:340:ARG:O	1.98	0.63
4:E:250:GLN:HA	4:E:253:VAL:HG12	1.81	0.63
3:C:56:LEU:O	7:C:502:HOH:O	2.16	0.63
2:B:232:ASN:OD1	2:B:236:GLN:NE2	2.32	0.62
2:B:321:GLN:HA	2:B:324:TYR:CD1	2.32	0.62
2:B:265:LEU:HD22	2:B:284:VAL:HG22	1.82	0.62
3:C:307:MET:HG2	3:C:316:MET:HE1	1.82	0.61
5:F:308:GLN:NE2	5:F:346:GLU:OE2	2.34	0.61
1:A:267:GLN:HB3	1:A:280:LEU:HD11	1.83	0.61
4:E:83:ARG:NH2	4:E:163:ILE:O	2.28	0.60
5:F:134:GLY:N	6:F:401:SO4:O1	2.24	0.60
2:B:195:ARG:NH1	7:B:501:HOH:O	2.34	0.59
3:C:102:TYR:N	7:C:503:HOH:O	2.35	0.59
3:C:267:GLN:HB3	3:C:280:LEU:HD11	1.84	0.59
1:A:206:LEU:HD12	1:A:229:LEU:HD11	1.85	0.58
3:C:265:LEU:HD22	3:C:282:ILE:HD11	1.86	0.58
4:E:220:GLU:OE2	4:E:256:GLN:NE2	2.30	0.58
5:F:324:TYR:HE1	5:F:351:LEU:HA	1.69	0.58
2:B:137:LYS:NZ	6:B:401:SO4:O3	2.36	0.58
2:B:195:ARG:NH2	3:C:161:ASP:OD1	2.37	0.58
4:D:220:GLU:OE1	7:D:502:HOH:O	2.17	0.57
2:B:233:SER:OG	2:B:236:GLN:HG2	2.05	0.56
4:D:129:VAL:HG21	4:D:141:LEU:HG	1.88	0.56
4:E:272:LYS:HG3	4:E:279:VAL:HG13	1.86	0.56
4:E:328:GLN:OE1	4:E:356:ARG:NH1	2.38	0.56
4:D:343:ASP:OD2	4:D:346:GLU:HG3	2.05	0.56
5:F:209:LEU:HD11	5:F:245:PHE:CD2	2.41	0.55
4:E:174:VAL:O	5:F:90:ARG:NH2	2.39	0.55
4:D:115:VAL:O	4:D:119:LEU:HD13	2.07	0.55
5:F:344:PRO:O	5:F:348:LYS:HG2	2.06	0.55
5:F:156:ILE:HB	5:F:174:VAL:HG12	1.90	0.54
5:F:254:ARG:NH2	7:F:501:HOH:O	2.36	0.54
4:D:169:HIS:CE1	4:D:174:VAL:H	2.25	0.54
4:E:11:LEU:HD22	4:E:19:LEU:HB2	1.90	0.54
1:A:220:GLU:OE2	1:A:256:GLN:HG2	2.08	0.53
5:F:132:PRO:HD3	5:F:232:ASN:OD1	2.08	0.53
2:B:235:VAL:HG13	2:B:300:ILE:HG22	1.90	0.53
4:E:137:LYS:N	6:E:401:SO4:O3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:LEU:HD13	3:C:212:ILE:HG12	1.92	0.52
4:E:265:LEU:HB3	4:E:282:ILE:HD11	1.91	0.52
3:C:307:MET:HG2	3:C:316:MET:CE	2.40	0.52
4:D:265:LEU:HD22	4:D:284:VAL:HG22	1.92	0.52
2:B:122:LYS:HD2	2:B:262:GLU:HB3	1.92	0.52
4:D:134:GLY:N	6:D:401:SO4:O2	2.41	0.52
4:E:265:LEU:HD22	4:E:284:VAL:HG22	1.91	0.52
4:D:145:ILE:HD11	4:D:167:HIS:CD2	2.44	0.51
2:B:197:ASP:OD2	3:C:18:ASP:OD2	2.29	0.51
5:F:220:GLU:OE1	5:F:256:GLN:NE2	2.33	0.51
2:B:6:GLN:O	2:B:9:THR:HG22	2.11	0.51
3:C:18:ASP:OD1	3:C:98:ARG:HG3	2.10	0.51
2:B:190:LEU:HD21	2:B:203:VAL:HG13	1.93	0.51
4:D:229:LEU:HD12	4:D:237:THR:HG23	1.93	0.50
3:C:43:LEU:HB3	3:C:47:ASP:HB2	1.93	0.50
2:B:206:LEU:HD23	2:B:212:ILE:HG12	1.94	0.50
4:D:59:GLN:NE2	4:D:180:GLY:O	2.45	0.50
4:E:155:HIS:CD2	4:E:173:VAL:HG23	2.47	0.49
3:C:103:LYS:HG3	7:C:503:HOH:O	2.12	0.49
4:D:145:ILE:HD11	4:D:167:HIS:CG	2.47	0.49
4:E:134:GLY:HA2	6:E:401:SO4:O1	2.12	0.49
3:C:83:ARG:HH11	3:C:83:ARG:HG3	1.77	0.49
5:F:267:GLN:HB3	5:F:280:LEU:HD11	1.94	0.49
4:D:106:SER:OG	4:D:109:GLU:HG3	2.13	0.49
5:F:115:VAL:HG21	5:F:315:GLY:O	2.13	0.49
1:A:115:VAL:HG11	1:A:284:VAL:HG11	1.95	0.48
4:D:240:ARG:O	4:D:244:VAL:HG23	2.13	0.48
4:E:18:ASP:OD1	4:E:98:ARG:HG2	2.13	0.48
4:D:221:THR:HG22	4:E:230:HIS:CE1	2.48	0.48
1:A:161:ASP:OD1	5:F:195:ARG:NH2	2.46	0.48
4:D:141:LEU:O	4:D:145:ILE:HG23	2.14	0.47
2:B:131:GLY:HA2	2:B:231:THR:O	2.14	0.47
5:F:3:ASN:OD1	5:F:4:MET:N	2.48	0.47
3:C:300:ILE:HA	3:C:303:ILE:HD13	1.96	0.47
1:A:124:ARG:CD	1:A:222:GLY:HA2	2.39	0.47
4:E:351:LEU:O	4:E:356:ARG:NH2	2.48	0.47
2:B:324:TYR:CZ	2:B:347:LEU:HD12	2.50	0.47
7:B:501:HOH:O	3:C:83:ARG:NH1	2.48	0.47
4:D:132:PRO:O	4:D:135:SER:HB3	2.14	0.47
2:B:291:ILE:HG23	2:B:303:ILE:HD12	1.96	0.46
3:C:294:LEU:HD13	3:C:302:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:O	1:A:350:MET:HG2	2.15	0.46
4:D:256:GLN:O	4:D:260:VAL:HG22	2.16	0.46
4:E:100:ILE:HG23	4:E:164:GLU:O	2.16	0.46
5:F:89:GLN:OE1	5:F:90:ARG:NE	2.44	0.46
2:B:254:ARG:NH1	2:B:298:ASP:HB2	2.31	0.45
4:E:240:ARG:O	4:E:240:ARG:HD3	2.17	0.45
5:F:307:MET:HG2	5:F:316:MET:CE	2.47	0.45
1:A:249:GLN:O	1:A:249:GLN:HG3	2.16	0.45
1:A:83:ARG:HB2	1:A:100:ILE:HD11	1.99	0.45
5:F:75:GLY:HA2	5:F:81:ARG:HA	1.98	0.44
3:C:179:VAL:HG21	3:C:186:PHE:CE1	2.52	0.44
3:C:83:ARG:NH1	3:C:83:ARG:HG3	2.32	0.44
4:D:333:THR:OG1	4:D:336:VAL:HG12	2.17	0.44
1:A:242:VAL:HG23	1:A:243:ASP:OD1	2.17	0.44
5:F:27:PRO:HB2	5:F:38:LEU:HD12	1.99	0.44
1:A:324:TYR:HB2	1:A:350:MET:HE3	2.00	0.44
5:F:27:PRO:HD3	5:F:43:LEU:HD11	1.99	0.44
5:F:58:GLU:OE2	5:F:61:LYS:NZ	2.44	0.44
3:C:11:LEU:HD22	3:C:19:LEU:HB2	2.00	0.44
2:B:29:ILE:HD12	2:B:38:LEU:HD21	2.00	0.43
4:D:122:MLY:O	4:D:224:LEU:HD22	2.19	0.43
4:D:267:GLN:HB3	4:D:280:LEU:HD11	2.00	0.43
5:F:332:ILE:HB	5:F:336:VAL:CG2	2.48	0.43
5:F:27:PRO:HB2	5:F:38:LEU:CD1	2.49	0.43
3:C:238:ILE:O	3:C:242:VAL:HG12	2.18	0.43
2:B:58:GLU:OE2	2:B:61:MLY:NZ	2.52	0.43
4:D:206:LEU:HB2	4:D:229:LEU:HD21	2.00	0.42
2:B:221:THR:HB	3:C:133:THR:OG1	2.19	0.42
4:E:149:ASN:OD1	4:E:172:CYS:HB2	2.18	0.42
3:C:250:GLN:N	3:C:251:PRO:HD2	2.33	0.42
4:E:209:LEU:HD12	4:E:209:LEU:H	1.84	0.42
4:D:332:ILE:HG22	4:D:336:VAL:HG11	2.01	0.42
4:E:206:LEU:HD12	4:E:229:LEU:HD11	2.00	0.42
4:E:235:VAL:HG13	4:E:300:ILE:HG22	2.01	0.42
1:A:55:ILE:HD11	1:A:97:PHE:CE1	2.55	0.42
4:E:288:ASN:ND2	7:E:502:HOH:O	2.53	0.42
1:A:100:ILE:HG23	1:A:164:GLU:O	2.20	0.42
4:E:82:PHE:CE2	4:E:99:VAL:HG12	2.54	0.42
4:E:179:VAL:HG21	4:E:186:PHE:CE1	2.54	0.42
4:E:76:ILE:HG21	4:E:79:LEU:HD12	2.02	0.42
5:F:144:ILE:O	5:F:148:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:GLY:CA	4:D:81:ARG:HG2	2.50	0.41
5:F:240:ARG:O	5:F:244:VAL:HG13	2.19	0.41
1:A:85:ASN:HD22	5:F:195:ARG:HB2	1.85	0.41
2:B:221:THR:HB	3:C:133:THR:HG1	1.85	0.41
4:D:205:GLU:OE2	4:D:230[A]:HIS:CE1	2.73	0.41
4:D:235:VAL:HG13	4:D:300:ILE:HG22	2.02	0.41
3:C:154:GLU:HB3	3:C:199:ASP:HB2	2.03	0.41
2:B:192:TYR:CD2	3:C:69:GLU:HG2	2.56	0.41
3:C:203:VAL:O	3:C:203:VAL:HG12	2.21	0.41
1:A:238:ILE:HG21	1:A:300:ILE:HD12	2.03	0.41
3:C:182:ASP:HB3	4:D:88:VAL:O	2.21	0.41
5:F:307:MET:HG2	5:F:316:MET:HE1	2.03	0.41
2:B:134:GLY:N	6:B:401:SO4:O3	2.50	0.40
4:D:134:GLY:HA2	6:D:401:SO4:O1	2.22	0.40
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.92	0.40
2:B:68:ASN:ND2	2:B:88:VAL:HG21	2.36	0.40
4:D:81:ARG:NH1	4:D:164:GLU:O	2.47	0.40
4:D:254:ARG:NH2	4:D:298:ASP:OD1	2.54	0.40
1:A:108:GLU:H	1:A:108:GLU:CD	2.25	0.40
2:B:320:ASN:O	2:B:324:TYR:CD1	2.75	0.40
2:B:221:THR:HG22	3:C:230:HIS:CE1	2.55	0.40
3:C:272:LYS:HG2	7:C:513:HOH:O	2.21	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	349/385 (91%)	343 (98%)	6 (2%)	0	100	100
2	B	351/385 (91%)	343 (98%)	8 (2%)	0	100	100
3	C	351/385 (91%)	343 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	350/385 (91%)	344 (98%)	6 (2%)	0	100	100
4	E	353/385 (92%)	348 (99%)	5 (1%)	0	100	100
5	F	350/385 (91%)	342 (98%)	8 (2%)	0	100	100
All	All	2104/2310 (91%)	2063 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	297/336 (88%)	296 (100%)	1 (0%)	92	96
2	B	274/336 (82%)	273 (100%)	1 (0%)	91	95
3	C	293/336 (87%)	293 (100%)	0	100	100
4	D	294/336 (88%)	289 (98%)	5 (2%)	60	78
4	E	301/336 (90%)	296 (98%)	5 (2%)	60	78
5	F	287/337 (85%)	286 (100%)	1 (0%)	92	96
All	All	1746/2017 (87%)	1733 (99%)	13 (1%)	84	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
2	B	72	LEU
4	D	59	GLN
4	D	72	LEU
4	D	135	SER
4	D	145	ILE
4	D	274	SER
4	E	72	LEU
4	E	73	SER
4	E	79	LEU

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Mol	Chain	Res	Type
4	E	240	ARG
4	E	311	GLN
5	F	72	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	59	GLN
4	D	252	GLN
4	D	321	GLN
5	F	308	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	MLY	A	272	1	9,10,11	0.69	0	6,11,13	0.96	0
4	MLY	E	170	4	9,10,11	0.75	0	6,11,13	0.76	0
2	MLY	B	49	2	9,10,11	0.70	0	6,11,13	0.83	0
4	MLY	E	122	4	9,10,11	0.44	0	6,11,13	0.97	0
3	MLY	C	122	3	9,10,11	0.61	0	6,11,13	0.57	0
1	MLY	A	61	1	9,10,11	0.47	0	6,11,13	0.90	0
2	MLY	B	61	2	9,10,11	0.43	0	6,11,13	0.83	0
3	MLY	C	61	3	9,10,11	0.69	0	6,11,13	0.85	0
4	MLY	D	170	4	9,10,11	0.59	0	6,11,13	0.81	0
5	MLY	F	63	5	9,10,11	0.61	0	6,11,13	0.66	0
4	MLY	D	122	4	9,10,11	0.68	0	6,11,13	0.68	0

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
1	MLY	A	272	1	-	0/8/9/11	-
4	MLY	E	170	4	-	1/8/9/11	-
2	MLY	B	49	2	-	0/8/9/11	-
4	MLY	E	122	4	-	0/8/9/11	-
3	MLY	C	122	3	-	0/8/9/11	-
1	MLY	A	61	1	-	2/8/9/11	-
2	MLY	B	61	2	-	0/8/9/11	-
3	MLY	C	61	3	-	1/8/9/11	-
4	MLY	D	170	4	-	3/8/9/11	-
5	MLY	F	63	5	-	0/8/9/11	-
4	MLY	D	122	4	-	0/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	170	MLY	O-C-CA-CB
4	D	170	MLY	N-CA-CB-CG
4	D	170	MLY	C-CA-CB-CG
1	A	61	MLY	CD-CE-NZ-CH2
1	A	61	MLY	CD-CE-NZ-CH1
3	C	61	MLY	CE-CD-CG-CB
4	D	170	MLY	CD-CE-NZ-CH2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	272	MLY	1	0
2	B	61	MLY	1	0
4	D	122	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
6	SO4	B	401	-	4,4,4	0.17	0	6,6,6	0.30	0
6	SO4	A	401	-	4,4,4	0.18	0	6,6,6	0.31	0
6	SO4	D	401	-	4,4,4	0.20	0	6,6,6	0.51	0
6	SO4	F	401	-	4,4,4	0.19	0	6,6,6	0.42	0
6	SO4	E	401	-	4,4,4	0.16	0	6,6,6	0.32	0
6	SO4	C	401	-	4,4,4	0.20	0	6,6,6	0.34	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.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	401	SO4	2	0
6	D	401	SO4	3	0
6	F	401	SO4	1	0
6	E	401	SO4	2	0

## 5.7 Other polymers [i](#)

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	351/385 (91%)	-0.29	0 100 100	43, 64, 97, 121	0
2	B	353/385 (91%)	-0.04	5 (1%) 75 75	45, 75, 135, 152	0
3	C	353/385 (91%)	-0.07	8 (2%) 60 59	43, 72, 108, 127	0
4	D	350/385 (90%)	-0.24	0 100 100	44, 63, 120, 149	0
4	E	354/385 (91%)	-0.30	1 (0%) 94 94	39, 61, 86, 114	0
5	F	351/385 (91%)	0.04	4 (1%) 80 81	50, 75, 107, 123	0
All	All	2112/2310 (91%)	-0.15	18 (0%) 84 84	39, 68, 114, 152	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	102	TYR	3.6
2	B	277	GLY	3.1
2	B	276	THR	3.0
5	F	311	GLN	2.8
5	F	13	ASN	2.8
3	C	310	GLY	2.7
2	B	331	HIS	2.7
5	F	337	GLY	2.6
3	C	78	GLY	2.6
4	E	2	ALA	2.5
3	C	343	ASP	2.5
5	F	345	ASP	2.4
2	B	347	LEU	2.3
2	B	274	SER	2.3
3	C	76	ILE	2.1
3	C	-1	SER	2.1
3	C	82	PHE	2.1
3	C	345	ASP	2.0



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

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
1	MLY	A	272	11/12	0.85	0.24	75,78,82,83	0
3	MLY	C	61	11/12	0.88	0.32	81,86,88,89	0
4	MLY	D	170	11/12	0.89	0.25	60,65,71,71	0
2	MLY	B	49	11/12	0.91	0.23	52,53,61,62	0
4	MLY	E	170	11/12	0.93	0.18	58,59,65,67	0
3	MLY	C	122	11/12	0.93	0.20	57,59,61,63	0
5	MLY	F	63	11/12	0.93	0.32	68,72,79,82	0
4	MLY	D	122	11/12	0.93	0.26	49,53,59,61	0
4	MLY	E	122	11/12	0.96	0.17	51,53,56,57	0
1	MLY	A	61	11/12	0.96	0.26	66,67,69,70	0
2	MLY	B	61	11/12	0.97	0.20	53,56,59,62	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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
6	SO4	B	401	5/5	0.97	0.15	50,52,61,67	0
6	SO4	E	401	5/5	0.97	0.13	32,33,38,45	0
6	SO4	F	401	5/5	0.98	0.09	47,50,59,62	0
6	SO4	A	401	5/5	0.99	0.11	28,35,39,40	0
6	SO4	D	401	5/5	0.99	0.10	28,35,43,45	0
6	SO4	C	401	5/5	0.99	0.08	36,43,51,55	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.