



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:38 PM GMT

PDB ID : 4FL4  
Title : Scaffoldin conformation and dynamics revealed by a ternary complex from the *Clostridium thermocellum* cellulosome  
Authors : Currie, M.A.; Adams, J.J.; Faucher, F.; Bayer, E.A.; Jia, Z.; Smith, S.P.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2012-06-14  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

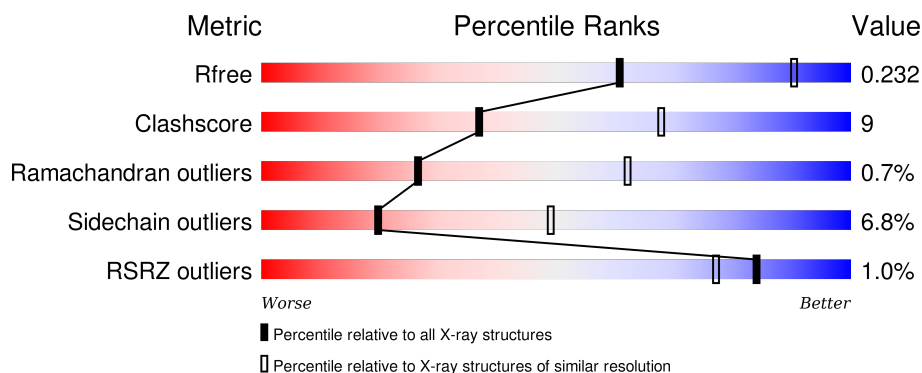
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	88	<div> <div>61%</div> <div>13%</div> <div>•</div> <div>23%</div> </div>
1	D	88	<div>2%</div> <div>49%</div> <div>23%</div> <div>•</div> <div>26%</div>

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Mol	Chain	Length	Quality of chain
2	E	187	
2	H	187	
2	K	187	
3	C	321	
3	F	321	
3	I	321	
3	L	321	

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
4	CA	C	402	-	-	-	X
5	SO4	F	410	-	-	-	X
5	SO4	F	412	-	-	-	X
5	SO4	F	413	-	-	X	-
5	SO4	K	203	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16313 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 Glycoside hydrolase family 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	68	Total	C	N	O	S	0	0	0
			497	308	88	100	1			
1	D	65	Total	C	N	O	S	0	0	0
			471	290	83	97	1			
1	G	67	Total	C	N	O	S	0	0	0
			500	308	88	103	1			
1	J	66	Total	C	N	O	S	0	0	0
			484	297	86	100	1			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP D1NID1
A	2	GLY	-	EXPRESSION TAG	UNP D1NID1
A	3	HIS	-	EXPRESSION TAG	UNP D1NID1
A	4	HIS	-	EXPRESSION TAG	UNP D1NID1
A	5	HIS	-	EXPRESSION TAG	UNP D1NID1
A	6	HIS	-	EXPRESSION TAG	UNP D1NID1
A	7	HIS	-	EXPRESSION TAG	UNP D1NID1
A	8	HIS	-	EXPRESSION TAG	UNP D1NID1
A	9	HIS	-	EXPRESSION TAG	UNP D1NID1
A	10	HIS	-	EXPRESSION TAG	UNP D1NID1
A	11	HIS	-	EXPRESSION TAG	UNP D1NID1
A	12	HIS	-	EXPRESSION TAG	UNP D1NID1
A	13	SER	-	EXPRESSION TAG	UNP D1NID1
A	14	SER	-	EXPRESSION TAG	UNP D1NID1
A	15	GLY	-	EXPRESSION TAG	UNP D1NID1
A	16	HIS	-	EXPRESSION TAG	UNP D1NID1
A	17	ILE	-	EXPRESSION TAG	UNP D1NID1
A	18	GLU	-	EXPRESSION TAG	UNP D1NID1
A	19	GLY	-	EXPRESSION TAG	UNP D1NID1
A	20	ARG	-	EXPRESSION TAG	UNP D1NID1
A	21	HIS	-	EXPRESSION TAG	UNP D1NID1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	EXPRESSION TAG	UNP D1NID1
D	1	MET	-	EXPRESSION TAG	UNP D1NID1
D	2	GLY	-	EXPRESSION TAG	UNP D1NID1
D	3	HIS	-	EXPRESSION TAG	UNP D1NID1
D	4	HIS	-	EXPRESSION TAG	UNP D1NID1
D	5	HIS	-	EXPRESSION TAG	UNP D1NID1
D	6	HIS	-	EXPRESSION TAG	UNP D1NID1
D	7	HIS	-	EXPRESSION TAG	UNP D1NID1
D	8	HIS	-	EXPRESSION TAG	UNP D1NID1
D	9	HIS	-	EXPRESSION TAG	UNP D1NID1
D	10	HIS	-	EXPRESSION TAG	UNP D1NID1
D	11	HIS	-	EXPRESSION TAG	UNP D1NID1
D	12	HIS	-	EXPRESSION TAG	UNP D1NID1
D	13	SER	-	EXPRESSION TAG	UNP D1NID1
D	14	SER	-	EXPRESSION TAG	UNP D1NID1
D	15	GLY	-	EXPRESSION TAG	UNP D1NID1
D	16	HIS	-	EXPRESSION TAG	UNP D1NID1
D	17	ILE	-	EXPRESSION TAG	UNP D1NID1
D	18	GLU	-	EXPRESSION TAG	UNP D1NID1
D	19	GLY	-	EXPRESSION TAG	UNP D1NID1
D	20	ARG	-	EXPRESSION TAG	UNP D1NID1
D	21	HIS	-	EXPRESSION TAG	UNP D1NID1
D	22	MET	-	EXPRESSION TAG	UNP D1NID1
G	1	MET	-	EXPRESSION TAG	UNP D1NID1
G	2	GLY	-	EXPRESSION TAG	UNP D1NID1
G	3	HIS	-	EXPRESSION TAG	UNP D1NID1
G	4	HIS	-	EXPRESSION TAG	UNP D1NID1
G	5	HIS	-	EXPRESSION TAG	UNP D1NID1
G	6	HIS	-	EXPRESSION TAG	UNP D1NID1
G	7	HIS	-	EXPRESSION TAG	UNP D1NID1
G	8	HIS	-	EXPRESSION TAG	UNP D1NID1
G	9	HIS	-	EXPRESSION TAG	UNP D1NID1
G	10	HIS	-	EXPRESSION TAG	UNP D1NID1
G	11	HIS	-	EXPRESSION TAG	UNP D1NID1
G	12	HIS	-	EXPRESSION TAG	UNP D1NID1
G	13	SER	-	EXPRESSION TAG	UNP D1NID1
G	14	SER	-	EXPRESSION TAG	UNP D1NID1
G	15	GLY	-	EXPRESSION TAG	UNP D1NID1
G	16	HIS	-	EXPRESSION TAG	UNP D1NID1
G	17	ILE	-	EXPRESSION TAG	UNP D1NID1
G	18	GLU	-	EXPRESSION TAG	UNP D1NID1
G	19	GLY	-	EXPRESSION TAG	UNP D1NID1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	20	ARG	-	EXPRESSION TAG	UNP D1NID1
G	21	HIS	-	EXPRESSION TAG	UNP D1NID1
G	22	MET	-	EXPRESSION TAG	UNP D1NID1
J	1	MET	-	EXPRESSION TAG	UNP D1NID1
J	2	GLY	-	EXPRESSION TAG	UNP D1NID1
J	3	HIS	-	EXPRESSION TAG	UNP D1NID1
J	4	HIS	-	EXPRESSION TAG	UNP D1NID1
J	5	HIS	-	EXPRESSION TAG	UNP D1NID1
J	6	HIS	-	EXPRESSION TAG	UNP D1NID1
J	7	HIS	-	EXPRESSION TAG	UNP D1NID1
J	8	HIS	-	EXPRESSION TAG	UNP D1NID1
J	9	HIS	-	EXPRESSION TAG	UNP D1NID1
J	10	HIS	-	EXPRESSION TAG	UNP D1NID1
J	11	HIS	-	EXPRESSION TAG	UNP D1NID1
J	12	HIS	-	EXPRESSION TAG	UNP D1NID1
J	13	SER	-	EXPRESSION TAG	UNP D1NID1
J	14	SER	-	EXPRESSION TAG	UNP D1NID1
J	15	GLY	-	EXPRESSION TAG	UNP D1NID1
J	16	HIS	-	EXPRESSION TAG	UNP D1NID1
J	17	ILE	-	EXPRESSION TAG	UNP D1NID1
J	18	GLU	-	EXPRESSION TAG	UNP D1NID1
J	19	GLY	-	EXPRESSION TAG	UNP D1NID1
J	20	ARG	-	EXPRESSION TAG	UNP D1NID1
J	21	HIS	-	EXPRESSION TAG	UNP D1NID1
J	22	MET	-	EXPRESSION TAG	UNP D1NID1

- Molecule 2 is a protein called Scaffolding dockerin binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1226	789	194	241	2			
2	E	165	Total	C	N	O	S	0	1	0
			1223	788	194	239	2			
2	H	165	Total	C	N	O	S	0	0	0
			1237	797	194	244	2			
2	K	164	Total	C	N	O	S	0	0	0
			1207	778	190	237	2			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP P71143

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ARG	-	EXPRESSION TAG	UNP P71143
B	3	GLY	-	EXPRESSION TAG	UNP P71143
B	4	SER	-	EXPRESSION TAG	UNP P71143
B	5	HIS	-	EXPRESSION TAG	UNP P71143
B	6	HIS	-	EXPRESSION TAG	UNP P71143
B	7	HIS	-	EXPRESSION TAG	UNP P71143
B	8	HIS	-	EXPRESSION TAG	UNP P71143
B	9	HIS	-	EXPRESSION TAG	UNP P71143
B	10	HIS	-	EXPRESSION TAG	UNP P71143
B	11	THR	-	EXPRESSION TAG	UNP P71143
B	12	ASP	-	EXPRESSION TAG	UNP P71143
B	13	LEU	-	EXPRESSION TAG	UNP P71143
B	187	PHE	TYR	CONFLICT	UNP P71143
E	1	MET	-	EXPRESSION TAG	UNP P71143
E	2	ARG	-	EXPRESSION TAG	UNP P71143
E	3	GLY	-	EXPRESSION TAG	UNP P71143
E	4	SER	-	EXPRESSION TAG	UNP P71143
E	5	HIS	-	EXPRESSION TAG	UNP P71143
E	6	HIS	-	EXPRESSION TAG	UNP P71143
E	7	HIS	-	EXPRESSION TAG	UNP P71143
E	8	HIS	-	EXPRESSION TAG	UNP P71143
E	9	HIS	-	EXPRESSION TAG	UNP P71143
E	10	HIS	-	EXPRESSION TAG	UNP P71143
E	11	THR	-	EXPRESSION TAG	UNP P71143
E	12	ASP	-	EXPRESSION TAG	UNP P71143
E	13	LEU	-	EXPRESSION TAG	UNP P71143
E	187	PHE	TYR	CONFLICT	UNP P71143
H	1	MET	-	EXPRESSION TAG	UNP P71143
H	2	ARG	-	EXPRESSION TAG	UNP P71143
H	3	GLY	-	EXPRESSION TAG	UNP P71143
H	4	SER	-	EXPRESSION TAG	UNP P71143
H	5	HIS	-	EXPRESSION TAG	UNP P71143
H	6	HIS	-	EXPRESSION TAG	UNP P71143
H	7	HIS	-	EXPRESSION TAG	UNP P71143
H	8	HIS	-	EXPRESSION TAG	UNP P71143
H	9	HIS	-	EXPRESSION TAG	UNP P71143
H	10	HIS	-	EXPRESSION TAG	UNP P71143
H	11	THR	-	EXPRESSION TAG	UNP P71143
H	12	ASP	-	EXPRESSION TAG	UNP P71143
H	13	LEU	-	EXPRESSION TAG	UNP P71143
H	187	PHE	TYR	CONFLICT	UNP P71143
K	1	MET	-	EXPRESSION TAG	UNP P71143

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Chain	Residue	Modelled	Actual	Comment	Reference
K	2	ARG	-	EXPRESSION TAG	UNP P71143
K	3	GLY	-	EXPRESSION TAG	UNP P71143
K	4	SER	-	EXPRESSION TAG	UNP P71143
K	5	HIS	-	EXPRESSION TAG	UNP P71143
K	6	HIS	-	EXPRESSION TAG	UNP P71143
K	7	HIS	-	EXPRESSION TAG	UNP P71143
K	8	HIS	-	EXPRESSION TAG	UNP P71143
K	9	HIS	-	EXPRESSION TAG	UNP P71143
K	10	HIS	-	EXPRESSION TAG	UNP P71143
K	11	THR	-	EXPRESSION TAG	UNP P71143
K	12	ASP	-	EXPRESSION TAG	UNP P71143
K	13	LEU	-	EXPRESSION TAG	UNP P71143
K	187	PHE	TYR	CONFLICT	UNP P71143

- Molecule 3 is a protein called Cellulosome anchoring protein cohesin region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	308	Total	C	N	O	S	0	0	0
			2260	1449	357	448	6			
3	F	308	Total	C	N	O	S	0	0	0
			2301	1471	363	461	6			
3	I	309	Total	C	N	O	S	1	0	0
			2290	1466	359	459	6			
3	L	306	Total	C	N	O	S	0	0	0
			2268	1451	354	457	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	INITIATING METHIONINE	UNP C7HJU1
C	314	LEU	-	EXPRESSION TAG	UNP C7HJU1
C	315	GLU	-	EXPRESSION TAG	UNP C7HJU1
C	316	HIS	-	EXPRESSION TAG	UNP C7HJU1
C	317	HIS	-	EXPRESSION TAG	UNP C7HJU1
C	318	HIS	-	EXPRESSION TAG	UNP C7HJU1
C	319	HIS	-	EXPRESSION TAG	UNP C7HJU1
C	320	HIS	-	EXPRESSION TAG	UNP C7HJU1
C	321	HIS	-	EXPRESSION TAG	UNP C7HJU1
F	1	MET	-	INITIATING METHIONINE	UNP C7HJU1
F	314	LEU	-	EXPRESSION TAG	UNP C7HJU1
F	315	GLU	-	EXPRESSION TAG	UNP C7HJU1
F	316	HIS	-	EXPRESSION TAG	UNP C7HJU1

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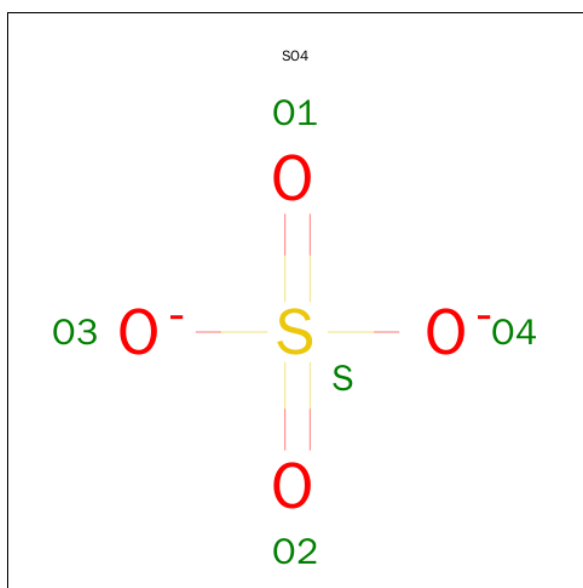
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Chain	Residue	Modelled	Actual	Comment	Reference
F	317	HIS	-	EXPRESSION TAG	UNP C7HJU1
F	318	HIS	-	EXPRESSION TAG	UNP C7HJU1
F	319	HIS	-	EXPRESSION TAG	UNP C7HJU1
F	320	HIS	-	EXPRESSION TAG	UNP C7HJU1
F	321	HIS	-	EXPRESSION TAG	UNP C7HJU1
I	1	MET	-	INITIATING METHIONINE	UNP C7HJU1
I	314	LEU	-	EXPRESSION TAG	UNP C7HJU1
I	315	GLU	-	EXPRESSION TAG	UNP C7HJU1
I	316	HIS	-	EXPRESSION TAG	UNP C7HJU1
I	317	HIS	-	EXPRESSION TAG	UNP C7HJU1
I	318	HIS	-	EXPRESSION TAG	UNP C7HJU1
I	319	HIS	-	EXPRESSION TAG	UNP C7HJU1
I	320	HIS	-	EXPRESSION TAG	UNP C7HJU1
I	321	HIS	-	EXPRESSION TAG	UNP C7HJU1
L	1	MET	-	INITIATING METHIONINE	UNP C7HJU1
L	314	LEU	-	EXPRESSION TAG	UNP C7HJU1
L	315	GLU	-	EXPRESSION TAG	UNP C7HJU1
L	316	HIS	-	EXPRESSION TAG	UNP C7HJU1
L	317	HIS	-	EXPRESSION TAG	UNP C7HJU1
L	318	HIS	-	EXPRESSION TAG	UNP C7HJU1
L	319	HIS	-	EXPRESSION TAG	UNP C7HJU1
L	320	HIS	-	EXPRESSION TAG	UNP C7HJU1
L	321	HIS	-	EXPRESSION TAG	UNP C7HJU1

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total Ca 2 2	0	0
4	J	2	Total Ca 2 2	0	0
4	D	2	Total Ca 2 2	0	0
4	I	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0
4	L	2	Total Ca 2 2	0	0
4	F	2	Total Ca 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	1	0
			5	4	1		
5	B	1	Total	O	S	1	0
			5	4	1		
5	B	1	Total	O	S	1	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	1	0
			5	4	1		
5	C	1	Total	O	S	1	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	1	0
			5	4	1		
5	C	1	Total	O	S	1	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	1	0
			5	4	1		
5	E	1	Total	O	S	1	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	1	0
			5	4	1		
5	E	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	1	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	1	0
			5	4	1		
5	H	1	Total	O	S	1	0
			5	4	1		
5	H	1	Total	O	S	1	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	1	0
			5	4	1		
5	H	1	Total	O	S	1	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	1	0
			5	4	1		
5	I	1	Total	O	S	1	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	1	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	1	0
			5	4	1		
5	K	1	Total	O	S	1	0
			5	4	1		
5	K	1	Total	O	S	1	0
			5	4	1		
5	K	1	Total	O	S	1	0
			5	4	1		
5	K	1	Total	O	S	1	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	1	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	1	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

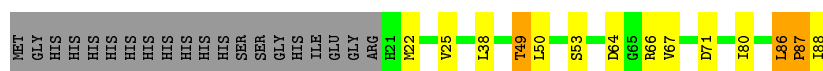
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	7	Total	O	0	0
			7	7		
6	C	6	Total	O	0	0
			6	6		
6	D	1	Total	O	0	0
			1	1		
6	E	3	Total	O	0	0
			3	3		
6	F	1	Total	O	0	0
			1	1		
6	G	2	Total	O	0	0
			2	2		
6	H	9	Total	O	0	0
			9	9		
6	I	4	Total	O	0	0
			4	4		
6	J	1	Total	O	0	0
			1	1		
6	K	2	Total	O	0	0
			2	2		
6	L	7	Total	O	0	0
			7	7		

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

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.

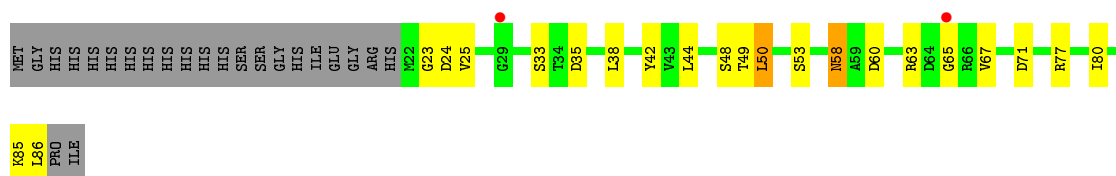
- Molecule 1: Glycoside hydrolase family 9

Chain A: 



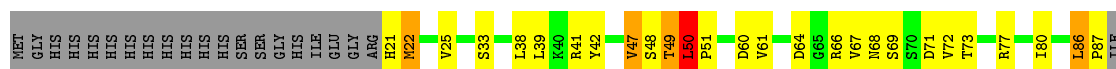
- Molecule 1: Glycoside hydrolase family 9

Chain D: 



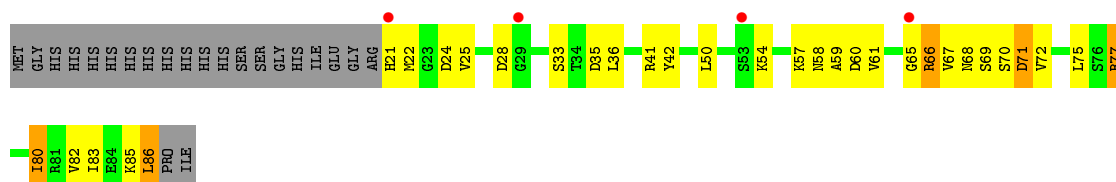
- Molecule 1: Glycoside hydrolase family 9

Chain G: 




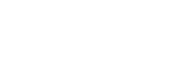
- Molecule 1: Glycoside hydrolase family 9

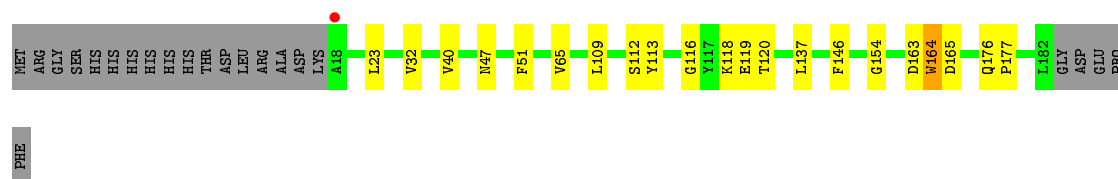
Chain J: 



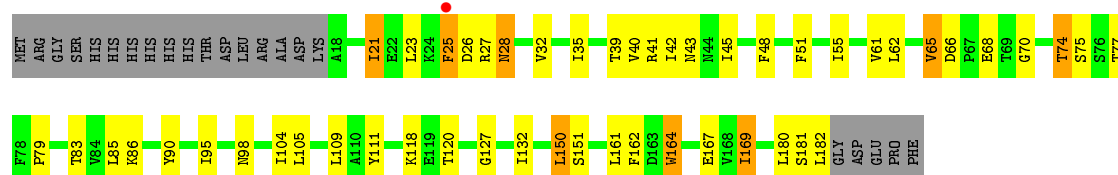
- Molecule 2: Scaffolding dockerin binding protein A

Chain B: 

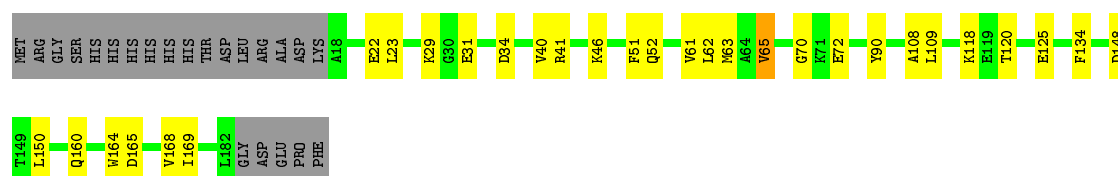




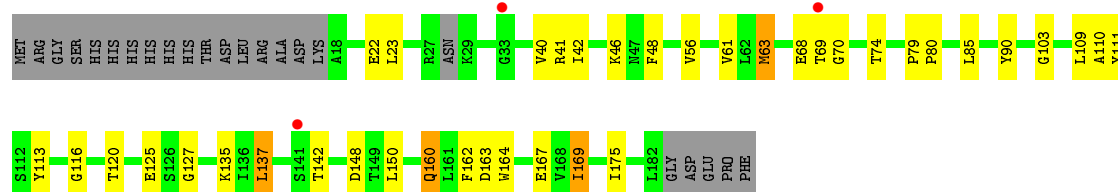
- Molecule 2: Scaffolding dockerin binding protein A



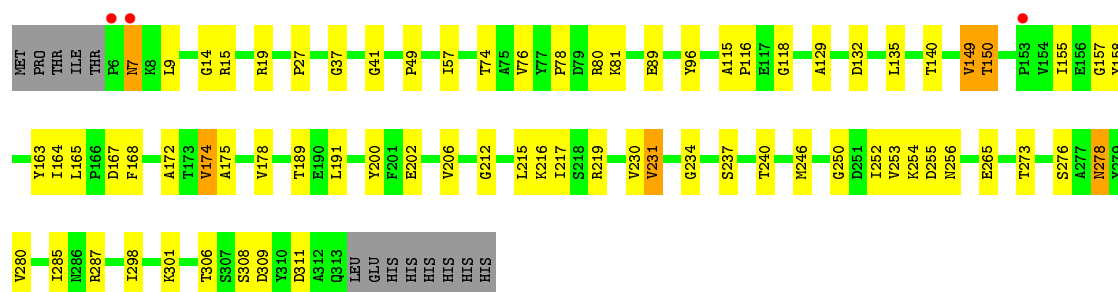
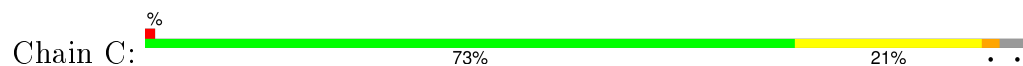
- Molecule 2: Scaffolding dockerin binding protein A



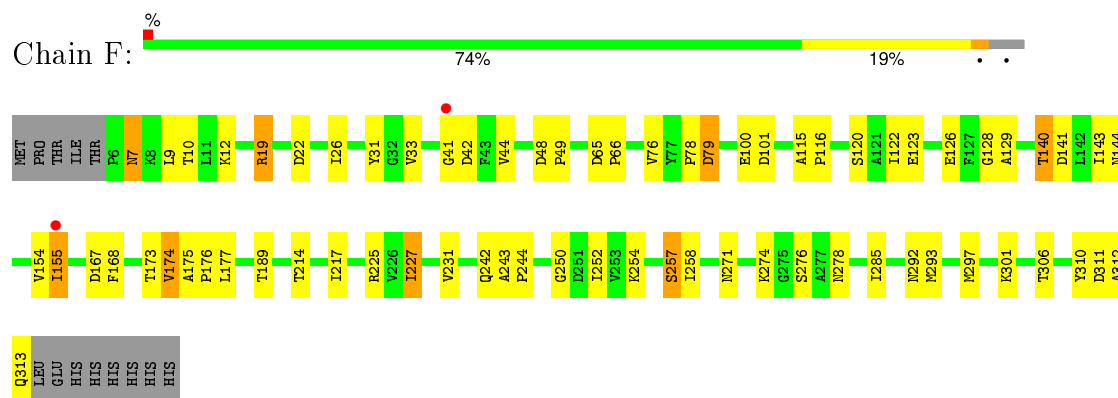
- Molecule 2: Scaffolding dockerin binding protein A



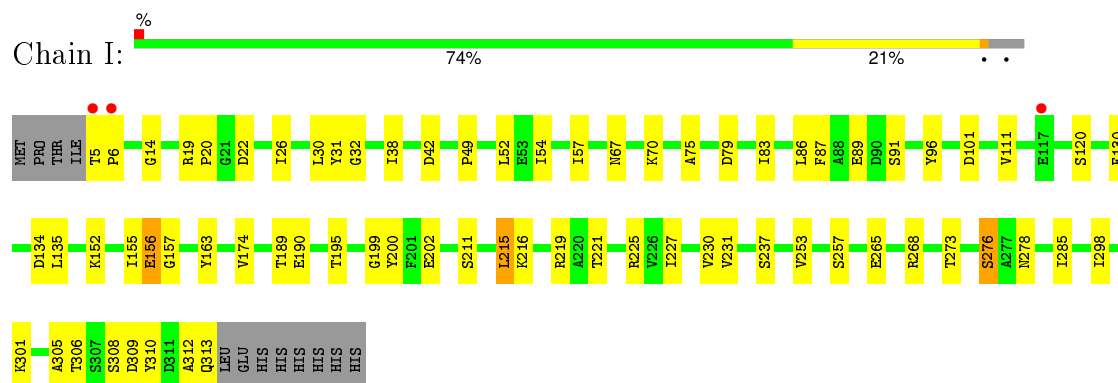
- Molecule 3: Cellulosome anchoring protein cohesin region



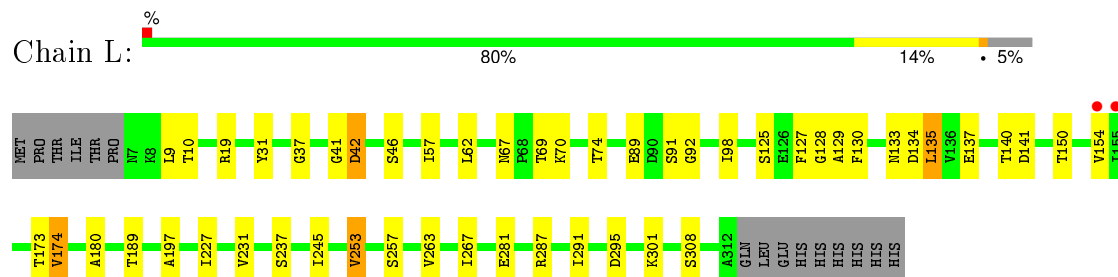
- Molecule 3: Cellulosome anchoring protein cohesin region



- Molecule 3: Cellulosome anchoring protein cohesin region



- Molecule 3: Cellulosome anchoring protein cohesin region





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.37Å 186.31Å 191.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.80 19.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.95-2.80) 99.5 (19.95-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.191 , 0.236 0.186 , 0.232	Depositor DCC
$R_{free}$ test set	5226 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 104323 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.38	0/501	0.63	0/684
1	D	0.37	0/473	0.65	0/645
1	G	0.41	0/504	0.65	0/686
1	J	0.35	0/487	0.61	0/664
2	B	0.46	0/1250	0.61	0/1704
2	E	0.41	0/1248	0.58	0/1705
2	H	0.46	0/1261	0.60	0/1716
2	K	0.41	0/1230	0.55	0/1676
3	C	0.47	0/2303	0.63	0/3148
3	F	0.46	0/2345	0.62	0/3201
3	I	0.48	0/2333	0.64	0/3186
3	L	0.42	0/2311	0.60	0/3159
All	All	0.44	0/16246	0.61	0/22174

There are no bond length outliers.

There are no bond angle outliers.

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	497	0	480	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	471	0	456	13	0
1	G	500	0	489	22	0
1	J	484	0	465	25	0
2	B	1226	0	1180	13	0
2	E	1223	0	1160	37	0
2	H	1237	0	1203	14	0
2	K	1207	0	1156	21	0
3	C	2260	0	2176	43	0
3	F	2301	0	2246	47	0
3	I	2290	0	2220	39	0
3	L	2268	0	2193	32	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	L	2	0	0	0	0
5	B	30	0	0	0	0
5	C	35	0	0	2	0
5	E	35	0	0	1	0
5	F	55	0	0	2	0
5	H	35	0	0	1	0
5	I	30	0	0	1	0
5	K	35	0	0	0	0
5	L	35	0	0	2	0
6	B	7	0	0	0	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	9	0	0	0	0
6	I	4	0	0	0	0
6	J	1	0	0	0	0
6	K	2	0	0	0	0
6	L	7	0	0	0	0
All	All	16313	0	15424	299	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 9.

The worst 5 of 299 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:A:86:LEU:O	1:A:88:ILE:N	1.97	0.97
1:G:49:THR:O	1:G:50:LEU:HB2	1.67	0.92
2:E:25[A]:PHE:N	2:E:25[A]:PHE:CD2	2.38	0.91
3:L:281:GLU:N	5:L:409:SO4:O3	2.04	0.90
2:E:25[A]:PHE:H	2:E:25[A]:PHE:HD2	1.15	0.89

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	66/88 (75%)	58 (88%)	6 (9%)	2 (3%)	5	18
1	D	63/88 (72%)	54 (86%)	9 (14%)	0	100	100
1	G	65/88 (74%)	60 (92%)	4 (6%)	1 (2%)	13	40
1	J	64/88 (73%)	54 (84%)	8 (12%)	2 (3%)	5	17
2	B	163/187 (87%)	156 (96%)	6 (4%)	1 (1%)	30	65
2	E	164/187 (88%)	158 (96%)	5 (3%)	1 (1%)	30	65
2	H	163/187 (87%)	158 (97%)	5 (3%)	0	100	100
2	K	160/187 (86%)	147 (92%)	12 (8%)	1 (1%)	30	65
3	C	306/321 (95%)	286 (94%)	19 (6%)	1 (0%)	46	79
3	F	306/321 (95%)	289 (94%)	15 (5%)	2 (1%)	26	62
3	I	307/321 (96%)	284 (92%)	19 (6%)	4 (1%)	15	44
3	L	304/321 (95%)	282 (93%)	22 (7%)	0	100	100
All	All	2131/2384 (89%)	1986 (93%)	130 (6%)	15 (1%)	26	62

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	PRO
3	I	152	LYS
3	F	7	ASN
1	J	58	ASN
2	E	32	VAL

### 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	53/79 (67%)	48 (91%)	5 (9%)	11	31
1	D	51/79 (65%)	46 (90%)	5 (10%)	10	28
1	G	56/79 (71%)	49 (88%)	7 (12%)	6	17
1	J	53/79 (67%)	49 (92%)	4 (8%)	17	43
2	B	126/156 (81%)	122 (97%)	4 (3%)	46	80
2	E	124/156 (80%)	109 (88%)	15 (12%)	6	18
2	H	129/156 (83%)	121 (94%)	8 (6%)	23	54
2	K	123/156 (79%)	114 (93%)	9 (7%)	17	44
3	C	233/266 (88%)	218 (94%)	15 (6%)	22	52
3	F	246/266 (92%)	231 (94%)	15 (6%)	23	55
3	I	241/266 (91%)	226 (94%)	15 (6%)	23	54
3	L	240/266 (90%)	228 (95%)	12 (5%)	30	64
All	All	1675/2004 (84%)	1561 (93%)	114 (7%)	20	49

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	174	VAL
1	G	49	THR
3	L	135	LEU
3	F	214	THR
3	F	257	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	144	ASN
1	J	68	ASN
3	I	313	GLN
2	E	28	ASN
1	J	21	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 16 are monoatomic - leaving 58 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	$\# Z  > 2$
5	SO4	B	201	-	4,4,4	0.36	0	6,6,6	0.67	0
5	SO4	B	202	-	4,4,4	0.30	0	6,6,6	0.30	0
5	SO4	B	203	-	4,4,4	0.38	0	6,6,6	0.23	0
5	SO4	B	204	-	4,4,4	0.07	0	6,6,6	0.45	0
5	SO4	B	205	-	4,4,4	0.17	0	6,6,6	0.38	0
5	SO4	B	206	-	4,4,4	0.17	0	6,6,6	0.26	0
5	SO4	C	403	-	4,4,4	0.44	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	C	404	-	4,4,4	0.27	0	6,6,6	0.42	0
5	SO4	C	405	-	4,4,4	0.12	0	6,6,6	0.20	0
5	SO4	C	406	-	4,4,4	0.12	0	6,6,6	0.21	0
5	SO4	C	407	-	4,4,4	0.28	0	6,6,6	0.20	0
5	SO4	C	408	-	4,4,4	0.22	0	6,6,6	0.16	0
5	SO4	C	409	-	4,4,4	0.32	0	6,6,6	0.80	0
5	SO4	E	201	-	4,4,4	0.32	0	6,6,6	0.32	0
5	SO4	E	202	-	4,4,4	0.31	0	6,6,6	0.29	0
5	SO4	E	203	-	4,4,4	0.22	0	6,6,6	0.28	0
5	SO4	E	204	-	4,4,4	0.14	0	6,6,6	0.17	0
5	SO4	E	205	-	4,4,4	0.21	0	6,6,6	0.68	0
5	SO4	E	206	-	4,4,4	0.22	0	6,6,6	0.31	0
5	SO4	E	207	-	4,4,4	0.06	0	6,6,6	0.18	0
5	SO4	F	403	-	4,4,4	0.17	0	6,6,6	0.18	0
5	SO4	F	404	-	4,4,4	0.64	0	6,6,6	0.58	0
5	SO4	F	405	-	4,4,4	0.19	0	6,6,6	0.27	0
5	SO4	F	406	-	4,4,4	0.24	0	6,6,6	0.30	0
5	SO4	F	407	-	4,4,4	0.18	0	6,6,6	0.31	0
5	SO4	F	408	-	4,4,4	0.36	0	6,6,6	0.13	0
5	SO4	F	409	-	4,4,4	0.22	0	6,6,6	0.21	0
5	SO4	F	410	-	4,4,4	0.11	0	6,6,6	0.25	0
5	SO4	F	411	-	4,4,4	0.22	0	6,6,6	0.13	0
5	SO4	F	412	-	4,4,4	0.20	0	6,6,6	0.44	0
5	SO4	F	413	-	4,4,4	0.26	0	6,6,6	0.17	0
5	SO4	H	201	-	4,4,4	0.15	0	6,6,6	0.25	0
5	SO4	H	202	-	4,4,4	0.48	0	6,6,6	0.64	0
5	SO4	H	203	-	4,4,4	0.35	0	6,6,6	0.20	0
5	SO4	H	204	-	4,4,4	0.10	0	6,6,6	0.21	0
5	SO4	H	205	-	4,4,4	0.31	0	6,6,6	0.29	0
5	SO4	H	206	-	4,4,4	0.30	0	6,6,6	0.41	0
5	SO4	H	207	-	4,4,4	0.17	0	6,6,6	0.21	0
5	SO4	I	403	-	4,4,4	0.66	0	6,6,6	0.64	0
5	SO4	I	404	-	4,4,4	0.24	0	6,6,6	0.21	0
5	SO4	I	405	-	4,4,4	0.23	0	6,6,6	0.17	0
5	SO4	I	406	-	4,4,4	0.20	0	6,6,6	0.51	0
5	SO4	I	407	-	4,4,4	0.32	0	6,6,6	0.27	0
5	SO4	I	408	-	4,4,4	0.08	0	6,6,6	0.30	0
5	SO4	K	201	-	4,4,4	0.36	0	6,6,6	0.31	0
5	SO4	K	202	-	4,4,4	0.19	0	6,6,6	0.26	0
5	SO4	K	203	-	4,4,4	0.22	0	6,6,6	0.17	0
5	SO4	K	204	-	4,4,4	0.10	0	6,6,6	0.20	0
5	SO4	K	205	-	4,4,4	0.11	0	6,6,6	0.32	0
5	SO4	K	206	-	4,4,4	0.14	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	K	207	-	4,4,4	0.18	0	6,6,6	0.19	0
5	SO4	L	403	-	4,4,4	0.21	0	6,6,6	0.20	0
5	SO4	L	404	-	4,4,4	0.44	0	6,6,6	0.51	0
5	SO4	L	405	-	4,4,4	0.26	0	6,6,6	0.27	0
5	SO4	L	406	-	4,4,4	0.12	0	6,6,6	0.25	0
5	SO4	L	407	-	4,4,4	0.19	0	6,6,6	0.20	0
5	SO4	L	408	-	4,4,4	0.11	0	6,6,6	0.25	0
5	SO4	L	409	-	4,4,4	0.13	0	6,6,6	0.27	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
5	SO4	B	201	-	-	0/0/0/0	0/0/0/0
5	SO4	B	202	-	-	0/0/0/0	0/0/0/0
5	SO4	B	203	-	-	0/0/0/0	0/0/0/0
5	SO4	B	204	-	-	0/0/0/0	0/0/0/0
5	SO4	B	205	-	-	0/0/0/0	0/0/0/0
5	SO4	B	206	-	-	0/0/0/0	0/0/0/0
5	SO4	C	403	-	-	0/0/0/0	0/0/0/0
5	SO4	C	404	-	-	0/0/0/0	0/0/0/0
5	SO4	C	405	-	-	0/0/0/0	0/0/0/0
5	SO4	C	406	-	-	0/0/0/0	0/0/0/0
5	SO4	C	407	-	-	0/0/0/0	0/0/0/0
5	SO4	C	408	-	-	0/0/0/0	0/0/0/0
5	SO4	C	409	-	-	0/0/0/0	0/0/0/0
5	SO4	E	201	-	-	0/0/0/0	0/0/0/0
5	SO4	E	202	-	-	0/0/0/0	0/0/0/0
5	SO4	E	203	-	-	0/0/0/0	0/0/0/0
5	SO4	E	204	-	-	0/0/0/0	0/0/0/0
5	SO4	E	205	-	-	0/0/0/0	0/0/0/0
5	SO4	E	206	-	-	0/0/0/0	0/0/0/0
5	SO4	E	207	-	-	0/0/0/0	0/0/0/0
5	SO4	F	403	-	-	0/0/0/0	0/0/0/0
5	SO4	F	404	-	-	0/0/0/0	0/0/0/0
5	SO4	F	405	-	-	0/0/0/0	0/0/0/0
5	SO4	F	406	-	-	0/0/0/0	0/0/0/0
5	SO4	F	407	-	-	0/0/0/0	0/0/0/0
5	SO4	F	408	-	-	0/0/0/0	0/0/0/0
5	SO4	F	409	-	-	0/0/0/0	0/0/0/0
5	SO4	F	410	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	F	411	-	-	0/0/0/0	0/0/0/0
5	SO4	F	412	-	-	0/0/0/0	0/0/0/0
5	SO4	F	413	-	-	0/0/0/0	0/0/0/0
5	SO4	H	201	-	-	0/0/0/0	0/0/0/0
5	SO4	H	202	-	-	0/0/0/0	0/0/0/0
5	SO4	H	203	-	-	0/0/0/0	0/0/0/0
5	SO4	H	204	-	-	0/0/0/0	0/0/0/0
5	SO4	H	205	-	-	0/0/0/0	0/0/0/0
5	SO4	H	206	-	-	0/0/0/0	0/0/0/0
5	SO4	H	207	-	-	0/0/0/0	0/0/0/0
5	SO4	I	403	-	-	0/0/0/0	0/0/0/0
5	SO4	I	404	-	-	0/0/0/0	0/0/0/0
5	SO4	I	405	-	-	0/0/0/0	0/0/0/0
5	SO4	I	406	-	-	0/0/0/0	0/0/0/0
5	SO4	I	407	-	-	0/0/0/0	0/0/0/0
5	SO4	I	408	-	-	0/0/0/0	0/0/0/0
5	SO4	K	201	-	-	0/0/0/0	0/0/0/0
5	SO4	K	202	-	-	0/0/0/0	0/0/0/0
5	SO4	K	203	-	-	0/0/0/0	0/0/0/0
5	SO4	K	204	-	-	0/0/0/0	0/0/0/0
5	SO4	K	205	-	-	0/0/0/0	0/0/0/0
5	SO4	K	206	-	-	0/0/0/0	0/0/0/0
5	SO4	K	207	-	-	0/0/0/0	0/0/0/0
5	SO4	L	403	-	-	0/0/0/0	0/0/0/0
5	SO4	L	404	-	-	0/0/0/0	0/0/0/0
5	SO4	L	405	-	-	0/0/0/0	0/0/0/0
5	SO4	L	406	-	-	0/0/0/0	0/0/0/0
5	SO4	L	407	-	-	0/0/0/0	0/0/0/0
5	SO4	L	408	-	-	0/0/0/0	0/0/0/0
5	SO4	L	409	-	-	0/0/0/0	0/0/0/0

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.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	404	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	405	SO4	1	0
5	E	202	SO4	1	0
5	F	413	SO4	2	0
5	H	202	SO4	1	0
5	I	405	SO4	1	0
5	L	407	SO4	1	0
5	L	409	SO4	1	0

## 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	68/88 (77%)	-0.25	0 100 100	59, 78, 98, 102	0
1	D	65/88 (73%)	-0.12	2 (3%) 52 40	64, 85, 100, 119	0
1	G	67/88 (76%)	-0.20	0 100 100	60, 75, 93, 97	0
1	J	66/88 (75%)	0.09	4 (6%) 25 15	72, 98, 119, 124	0
2	B	165/187 (88%)	-0.38	1 (0%) 90 86	51, 68, 91, 115	0
2	E	165/187 (88%)	-0.30	1 (0%) 90 86	53, 74, 100, 117	0
2	H	165/187 (88%)	-0.45	0 100 100	52, 67, 91, 108	0
2	K	164/187 (87%)	-0.21	3 (1%) 71 61	58, 79, 104, 116	0
3	C	308/321 (95%)	-0.48	3 (0%) 84 77	50, 63, 81, 112	0
3	F	308/321 (95%)	-0.37	2 (0%) 90 86	53, 66, 87, 121	0
3	I	309/321 (96%)	-0.46	3 (0%) 84 77	51, 62, 81, 115	1 (0%)
3	L	306/321 (95%)	-0.39	2 (0%) 89 84	57, 70, 90, 113	0
All	All	2156/2384 (90%)	-0.36	21 (0%) 84 77	50, 69, 99, 124	1 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	69	THR	3.5
3	I	5	THR	3.5
1	J	21	HIS	3.0
3	C	153	PRO	2.9
2	K	33	GLY	2.5

### 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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	K	203	5/5	0.66	0.38	16.95	58,73,76,85	1
5	SO4	F	412	5/5	0.83	0.47	4.35	61,64,66,66	4
5	SO4	F	410	5/5	0.71	0.29	2.62	91,94,97,100	1
4	CA	C	402	1/1	0.93	0.25	2.14	63,63,63,63	0
5	SO4	F	413	5/5	0.86	0.34	1.95	75,77,82,86	3
4	CA	F	401	1/1	0.99	0.21	1.81	59,59,59,59	0
4	CA	I	401	1/1	0.97	0.22	1.71	62,62,62,62	0
5	SO4	B	203	5/5	0.92	0.18	0.63	67,68,75,76	1
4	CA	L	401	1/1	0.99	0.21	0.61	68,68,68,68	0
5	SO4	C	405	5/5	0.90	0.22	0.44	66,69,82,84	1
5	SO4	I	403	5/5	0.94	0.20	0.26	51,52,56,59	1
5	SO4	I	406	5/5	0.82	0.18	-0.10	65,76,79,80	1
4	CA	I	402	1/1	0.98	0.15	-0.11	64,64,64,64	0
5	SO4	F	404	5/5	0.90	0.16	-0.18	53,55,59,63	1
4	CA	C	401	1/1	0.97	0.16	-0.22	64,64,64,64	0
5	SO4	K	206	5/5	0.93	0.15	-0.33	88,95,103,107	2
5	SO4	C	403	5/5	0.94	0.14	-0.44	52,58,62,67	1
4	CA	L	402	1/1	0.98	0.13	-0.76	72,72,72,72	0
5	SO4	L	404	5/5	0.95	0.12	-0.83	58,65,67,75	1
4	CA	A	101	1/1	0.98	0.13	-0.84	81,81,81,81	0
4	CA	F	402	1/1	0.96	0.13	-1.09	69,69,69,69	0
4	CA	G	101	1/1	0.96	0.15	-1.21	72,72,72,72	0
4	CA	A	102	1/1	0.91	0.10	-1.39	86,86,86,86	0
4	CA	G	102	1/1	0.95	0.09	-1.39	89,89,89,89	0
4	CA	J	102	1/1	0.96	0.10	-1.45	110,110,110,110	0
4	CA	J	101	1/1	0.97	0.13	-1.87	102,102,102,102	0
4	CA	D	101	1/1	0.95	0.10	-2.22	90,90,90,90	0
4	CA	D	102	1/1	0.93	0.09	-2.43	97,97,97,97	0
5	SO4	C	406	5/5	0.84	0.31	-	73,74,78,78	1
5	SO4	B	201	5/5	0.96	0.13	-	61,67,70,73	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	I	407	5/5	0.99	0.10	-	60,61,68,69	2
5	SO4	H	202	5/5	0.93	0.13	-	54,61,62,63	1
5	SO4	B	205	5/5	0.87	0.25	-	64,65,68,75	1
5	SO4	B	202	5/5	0.96	0.13	-	65,66,67,67	1
5	SO4	H	206	5/5	0.93	0.30	-	62,67,70,78	1
5	SO4	C	409	5/5	0.72	0.28	-	64,73,79,82	1
5	SO4	H	201	5/5	0.92	0.25	-	61,62,66,70	2
5	SO4	L	405	5/5	0.97	0.13	-	61,67,70,72	2
5	SO4	E	203	5/5	0.95	0.16	-	67,68,73,81	1
5	SO4	B	204	5/5	0.81	0.49	-	76,77,79,86	2
5	SO4	L	409	5/5	0.93	0.45	-	91,93,99,104	4
5	SO4	K	201	5/5	0.97	0.11	-	63,68,72,76	1
5	SO4	I	405	5/5	0.92	0.25	-	60,61,66,71	2
5	SO4	E	202	5/5	0.87	0.28	-	65,70,71,76	2
5	SO4	H	205	5/5	0.90	0.27	-	73,76,87,94	1
5	SO4	I	404	5/5	0.91	0.24	-	67,69,77,85	1
5	SO4	H	207	5/5	0.93	0.16	-	80,80,87,87	2
5	SO4	F	408	5/5	0.99	0.14	-	58,58,61,68	1
5	SO4	F	403	5/5	0.88	0.21	-	72,79,82,88	2
5	SO4	E	204	5/5	0.88	0.44	-	91,93,102,102	2
5	SO4	C	408	5/5	0.89	0.21	-	65,68,72,76	1
5	SO4	F	411	5/5	0.89	0.25	-	71,74,80,82	2
5	SO4	K	205	5/5	0.82	0.27	-	77,83,87,89	1
5	SO4	K	202	5/5	0.84	0.26	-	69,79,80,85	1
5	SO4	F	409	5/5	0.91	0.24	-	79,81,87,90	2
5	SO4	E	205	5/5	0.93	0.33	-	82,83,85,89	1
5	SO4	H	203	5/5	0.92	0.14	-	60,64,67,73	1
5	SO4	C	407	5/5	0.98	0.20	-	59,62,67,68	2
5	SO4	F	407	5/5	0.79	0.30	-	70,72,79,80	2
5	SO4	H	204	5/5	0.88	0.24	-	78,81,94,98	1
5	SO4	K	207	5/5	0.96	0.32	-	96,104,108,109	2
5	SO4	L	406	5/5	0.95	0.18	-	61,62,68,70	1
5	SO4	B	206	5/5	0.91	0.14	-	91,98,101,104	1
5	SO4	C	404	5/5	0.96	0.21	-	50,54,56,57	2
5	SO4	L	408	5/5	0.90	0.23	-	68,78,81,85	1
5	SO4	I	408	5/5	0.85	0.25	-	64,68,78,80	1
5	SO4	L	403	5/5	0.86	0.29	-	76,78,80,84	1
5	SO4	F	406	5/5	0.85	0.27	-	77,80,85,91	1
5	SO4	E	201	5/5	0.96	0.13	-	58,60,65,70	2
5	SO4	E	207	5/5	0.97	0.32	-	73,76,77,77	1
5	SO4	K	204	5/5	0.84	0.39	-	73,80,82,87	1
5	SO4	L	407	5/5	0.93	0.35	-	75,78,79,85	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	F	405	5/5	0.91	0.24	-	62,65,68,71	2
5	SO4	E	206	5/5	0.92	0.30	-	70,72,72,73	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.