



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:30 AM UTC

PDB ID : 4FL4 / pdb_00004fl4
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

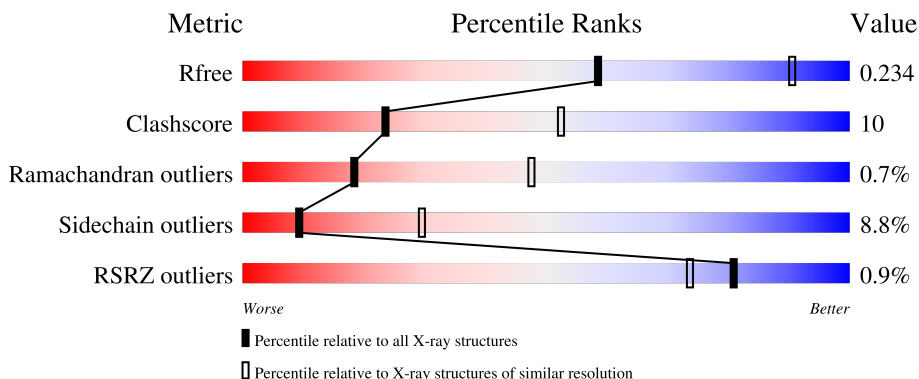
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	88	 53% 19% 5% 23%
1	D	88	 41% 27% 6% 26%
1	G	88	 44% 25% 5% 24%
1	J	88	 36% 31% 8% 25%
2	B	187	 73% 16% 12%

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Mol	Chain	Length	Quality of chain
2	E	187	<p>%</p> <p>59% 25% • 12%</p>
2	H	187	<p>%</p> <p>68% 19% • 12%</p>
2	K	187	<p>2%</p> <p>66% 19% • 12%</p>
3	C	321	<p>%</p> <p>71% 22% • •</p>
3	F	321	<p>72% 20% • •</p>
3	I	321	<p>%</p> <p>71% 24% • •</p>
3	L	321	<p>76% 18% • 5%</p>

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
5	SO4	F	413	-	-	X	-

2 Entry composition i

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

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

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

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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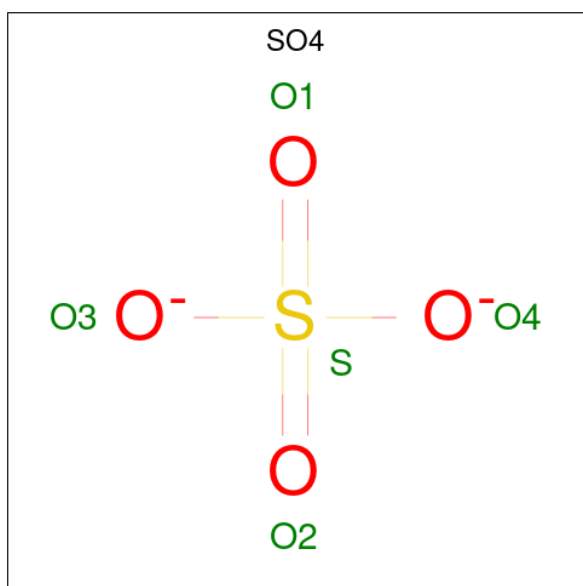
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Chain	Residue	Modelled	Actual	Comment	Reference
F	317	HIS	-	expression tag	UNP C7HJU1
F	318	HIS	-	expression tag	UNP C7HJU1
F	319	HIS	-	expression tag	UNP C7HJU1
F	320	HIS	-	expression tag	UNP C7HJU1
F	321	HIS	-	expression tag	UNP C7HJU1
I	1	MET	-	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 (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	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 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	1	0
5	H	1	Total 5	O 4	S 1	1	0
5	H	1	Total 5	O 4	S 1	0	0
5	I	1	Total 5	O 4	S 1	1	0
5	I	1	Total 5	O 4	S 1	1	0
5	I	1	Total 5	O 4	S 1	0	0
5	I	1	Total 5	O 4	S 1	1	0
5	I	1	Total 5	O 4	S 1	0	0
5	I	1	Total 5	O 4	S 1	1	0
5	K	1	Total 5	O 4	S 1	1	0
5	K	1	Total 5	O 4	S 1	1	0
5	K	1	Total 5	O 4	S 1	1	0
5	K	1	Total 5	O 4	S 1	1	0
5	K	1	Total 5	O 4	S 1	0	0
5	K	1	Total 5	O 4	S 1	0	0
5	K	1	Total 5	O 4	S 1	0	0
5	L	1	Total 5	O 4	S 1	1	0
5	L	1	Total 5	O 4	S 1	0	0
5	L	1	Total 5	O 4	S 1	0	0
5	L	1	Total 5	O 4	S 1	1	0

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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, 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.

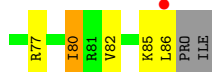
- Molecule 1: Glycoside hydrolase family 9

Chain A: 




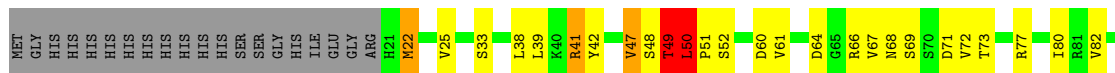
- Molecule 1: Glycoside hydrolase family 9

Chain D: 



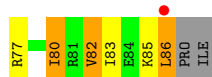
- Molecule 1: Glycoside hydrolase family 9

Chain G: 

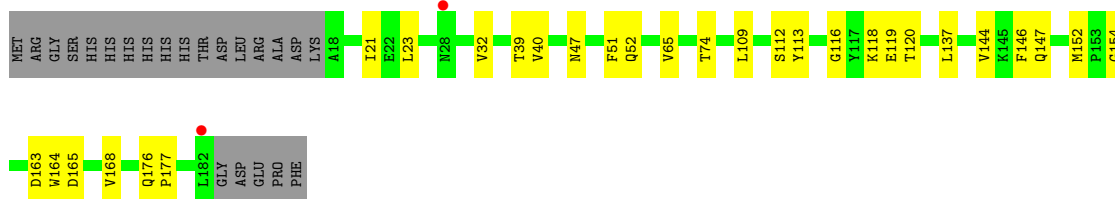


- Molecule 1: Glycoside hydrolase family 9

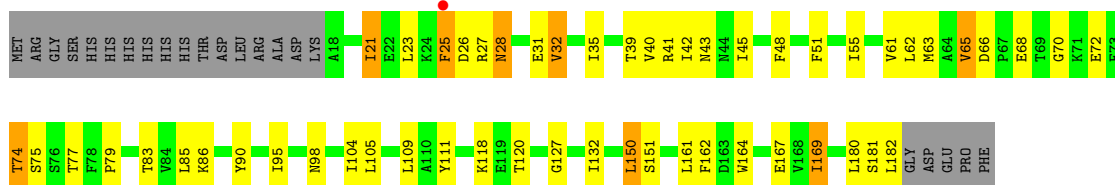
Chain J: 



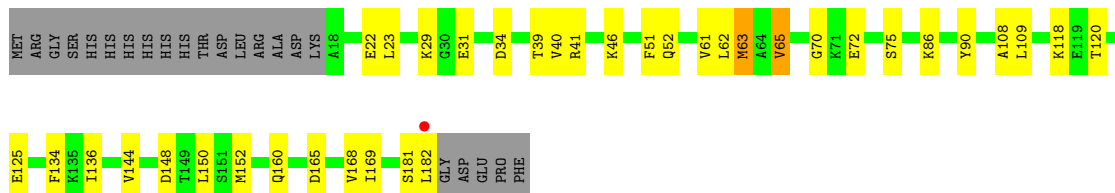
- Molecule 2: Scaffolding dockerin binding protein A



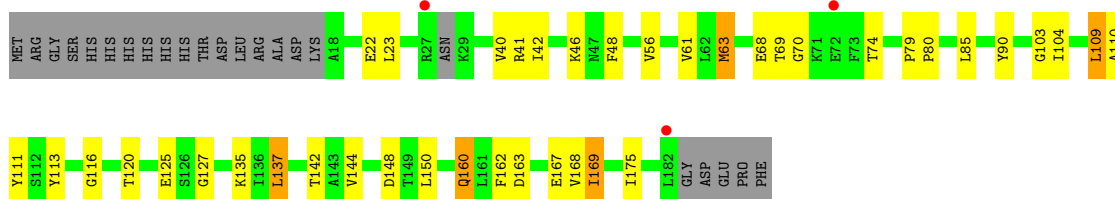
- Molecule 2: Scaffolding dockerin binding protein A



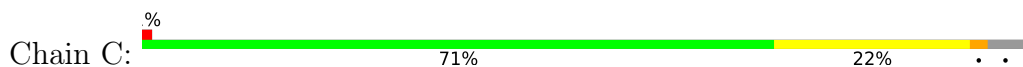
- Molecule 2: Scaffolding dockerin binding protein A

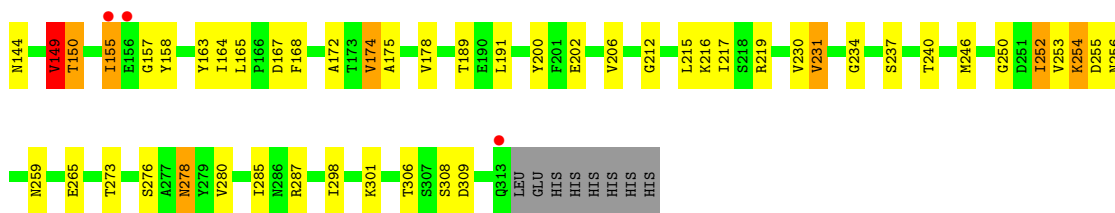


- Molecule 2: Scaffolding dockerin binding protein A

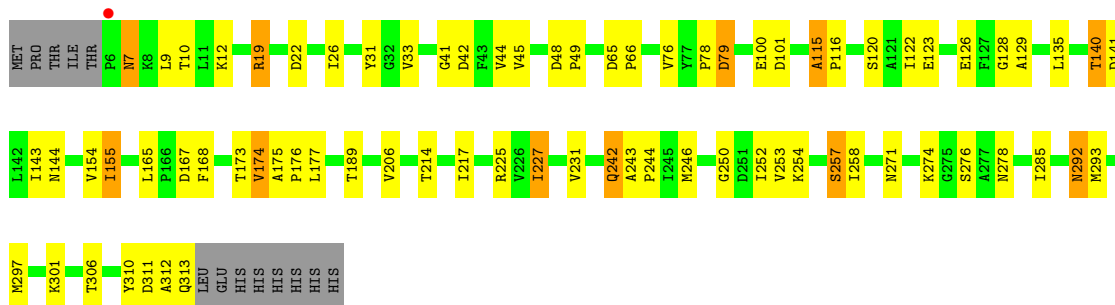


- Molecule 3: Cellulosome anchoring protein cohesin region

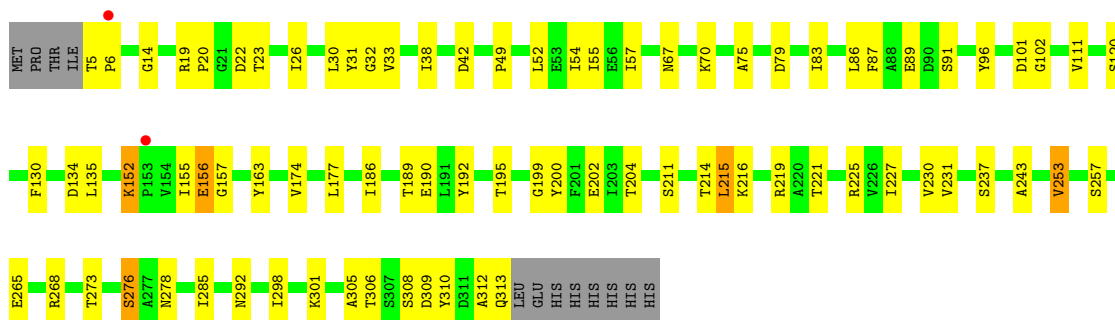




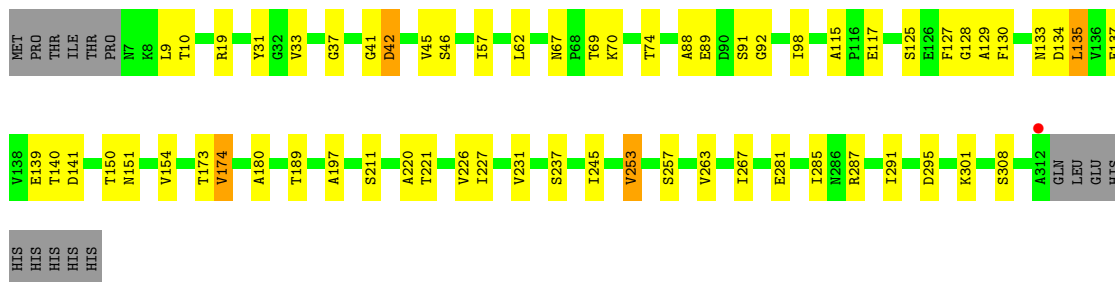
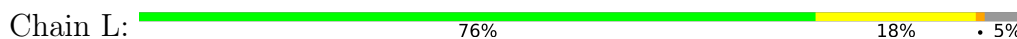
• Molecule 3: Cellulosome anchoring protein cohesin region



• Molecule 3: Cellulosome anchoring protein cohesin region



• Molecule 3: Cellulosome anchoring protein cohesin region



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 99.2 (19.95-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.79Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.191 , 0.236 0.189 , 0.234	Depositor DCC
R_{free} test set	5224 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtrriage
Anisotropy	0.303	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.029 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16313	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.55	0/501	0.95	2/684 (0.3%)
1	D	0.54	0/473	1.02	4/645 (0.6%)
1	G	0.58	0/504	1.08	4/686 (0.6%)
1	J	0.46	0/487	0.97	2/664 (0.3%)
2	B	0.57	0/1250	0.94	0/1704
2	E	0.50	0/1248	0.88	0/1705
2	H	0.55	0/1261	0.89	0/1716
2	K	0.50	0/1230	0.87	1/1676 (0.1%)
3	C	0.60	0/2303	0.97	10/3148 (0.3%)
3	F	0.56	0/2345	0.95	5/3201 (0.2%)
3	I	0.61	0/2333	1.02	9/3186 (0.3%)
3	L	0.52	0/2311	0.96	5/3159 (0.2%)
All	All	0.56	0/16246	0.96	42/22174 (0.2%)

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	152	LYS	CA-C-N	10.55	133.03	119.84
3	I	152	LYS	C-N-CA	10.55	133.03	119.84
3	F	115	ALA	CA-C-N	8.66	128.60	119.85
3	F	115	ALA	C-N-CA	8.66	128.60	119.85
3	I	33	VAL	CA-C-N	7.70	127.71	119.78

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	13	0
1	D	471	0	456	14	0
1	G	500	0	489	23	0
1	J	484	0	465	27	0
2	B	1226	0	1180	14	0
2	E	1223	0	1160	40	0
2	H	1237	0	1203	18	0
2	K	1207	0	1156	22	0
3	C	2260	0	2176	46	0
3	F	2301	0	2246	49	0
3	I	2290	0	2220	40	0
3	L	2268	0	2193	35	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	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	2	0	0	0	0
6	L	7	0	0	0	0
All	All	16313	0	15424	324	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 10.

The worst 5 of 324 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%)	3	12
1	D	63/88 (72%)	54 (86%)	9 (14%)	0	100	100
1	G	65/88 (74%)	60 (92%)	4 (6%)	1 (2%)	8	28
1	J	64/88 (73%)	54 (84%)	8 (12%)	2 (3%)	3	12
2	B	163/187 (87%)	156 (96%)	6 (4%)	1 (1%)	21	51
2	E	164/187 (88%)	158 (96%)	5 (3%)	1 (1%)	21	51
2	H	163/187 (87%)	158 (97%)	5 (3%)	0	100	100
2	K	160/187 (86%)	147 (92%)	12 (8%)	1 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	306/321 (95%)	286 (94%)	19 (6%)	1 (0%)	36	66
3	F	306/321 (95%)	289 (94%)	15 (5%)	2 (1%)	18	47
3	I	307/321 (96%)	284 (92%)	19 (6%)	4 (1%)	9	31
3	L	304/321 (95%)	282 (93%)	22 (7%)	0	100	100
All	All	2131/2384 (89%)	1986 (93%)	130 (6%)	15 (1%)	18	47

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	53/79 (67%)	46 (87%)	7 (13%)	4	14
1	D	51/79 (65%)	42 (82%)	9 (18%)	2	7
1	G	56/79 (71%)	48 (86%)	8 (14%)	3	11
1	J	53/79 (67%)	47 (89%)	6 (11%)	5	19
2	B	126/156 (81%)	117 (93%)	9 (7%)	13	39
2	E	124/156 (80%)	110 (89%)	14 (11%)	5	19
2	H	129/156 (83%)	117 (91%)	12 (9%)	8	27
2	K	123/156 (79%)	112 (91%)	11 (9%)	9	29
3	C	233/266 (88%)	216 (93%)	17 (7%)	13	38
3	F	246/266 (92%)	228 (93%)	18 (7%)	13	38
3	I	241/266 (91%)	220 (91%)	21 (9%)	9	30
3	L	240/266 (90%)	224 (93%)	16 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1675/2004 (84%)	1527 (91%)	148 (9%)	9 29

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	25	VAL
3	L	231	VAL
1	J	82	VAL
2	K	168	VAL
2	E	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	313	GLN
1	J	21	HIS
1	J	68	ASN
3	F	144	ASN
3	F	256	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 oligosaccharides 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	I	404	-	4,4,4	0.25	0	6,6,6	0.20	0
5	SO4	B	204	-	4,4,4	0.26	0	6,6,6	0.38	0
5	SO4	I	403	-	4,4,4	0.21	0	6,6,6	0.61	0
5	SO4	H	201	-	4,4,4	0.33	0	6,6,6	0.34	0
5	SO4	K	206	-	4,4,4	0.22	0	6,6,6	0.21	0
5	SO4	H	202	-	4,4,4	0.28	0	6,6,6	0.82	0
5	SO4	E	207	-	4,4,4	0.30	0	6,6,6	0.13	0
5	SO4	F	407	-	4,4,4	0.28	0	6,6,6	0.28	0
5	SO4	F	406	-	4,4,4	0.27	0	6,6,6	0.25	0
5	SO4	B	206	-	4,4,4	0.22	0	6,6,6	0.29	0
5	SO4	K	203	-	4,4,4	0.36	0	6,6,6	0.23	0
5	SO4	F	410	-	4,4,4	0.26	0	6,6,6	0.19	0
5	SO4	H	205	-	4,4,4	0.31	0	6,6,6	0.25	0
5	SO4	L	408	-	4,4,4	0.29	0	6,6,6	0.23	0
5	SO4	H	204	-	4,4,4	0.24	0	6,6,6	0.15	0
5	SO4	F	409	-	4,4,4	0.31	0	6,6,6	0.16	0
5	SO4	F	413	-	4,4,4	0.22	0	6,6,6	0.19	0
5	SO4	F	403	-	4,4,4	0.25	0	6,6,6	0.16	0
5	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.51	0
5	SO4	L	405	-	4,4,4	0.19	0	6,6,6	0.26	0
5	SO4	C	408	-	4,4,4	0.25	0	6,6,6	0.24	0
5	SO4	B	203	-	4,4,4	0.27	0	6,6,6	0.22	0
5	SO4	L	407	-	4,4,4	0.24	0	6,6,6	0.23	0
5	SO4	B	205	-	4,4,4	0.25	0	6,6,6	0.30	0
5	SO4	K	202	-	4,4,4	0.26	0	6,6,6	0.34	0
5	SO4	K	201	-	4,4,4	0.19	0	6,6,6	0.32	0
5	SO4	I	405	-	4,4,4	0.25	0	6,6,6	0.17	0
5	SO4	E	201	-	4,4,4	0.22	0	6,6,6	0.38	0
5	SO4	C	407	-	4,4,4	0.25	0	6,6,6	0.25	0
5	SO4	L	404	-	4,4,4	0.15	0	6,6,6	0.36	0
5	SO4	C	409	-	4,4,4	0.21	0	6,6,6	0.58	0
5	SO4	I	408	-	4,4,4	0.27	0	6,6,6	0.28	0
5	SO4	H	206	-	4,4,4	0.25	0	6,6,6	0.34	0
5	SO4	C	405	-	4,4,4	0.30	0	6,6,6	0.32	0
5	SO4	C	404	-	4,4,4	0.22	0	6,6,6	0.37	0
5	SO4	B	202	-	4,4,4	0.19	0	6,6,6	0.27	0
5	SO4	F	408	-	4,4,4	0.20	0	6,6,6	0.13	0
5	SO4	K	205	-	4,4,4	0.33	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	E	205	-	4,4,4	0.28	0	6,6,6	0.52	0
5	SO4	K	204	-	4,4,4	0.31	0	6,6,6	0.25	0
5	SO4	B	201	-	4,4,4	0.23	0	6,6,6	0.67	0
5	SO4	E	204	-	4,4,4	0.24	0	6,6,6	0.19	0
5	SO4	H	203	-	4,4,4	0.21	0	6,6,6	0.24	0
5	SO4	L	406	-	4,4,4	0.29	0	6,6,6	0.42	0
5	SO4	H	207	-	4,4,4	0.31	0	6,6,6	0.15	0
5	SO4	I	406	-	4,4,4	0.19	0	6,6,6	0.42	0
5	SO4	C	406	-	4,4,4	0.26	0	6,6,6	0.18	0
5	SO4	F	411	-	4,4,4	0.22	0	6,6,6	0.15	0
5	SO4	F	412	-	4,4,4	0.30	0	6,6,6	0.52	0
5	SO4	L	409	-	4,4,4	0.31	0	6,6,6	0.22	0
5	SO4	E	202	-	4,4,4	0.19	0	6,6,6	0.28	0
5	SO4	F	405	-	4,4,4	0.24	0	6,6,6	0.26	0
5	SO4	I	407	-	4,4,4	0.22	0	6,6,6	0.24	0
5	SO4	K	207	-	4,4,4	0.27	0	6,6,6	0.21	0
5	SO4	F	404	-	4,4,4	0.26	0	6,6,6	0.76	0
5	SO4	E	206	-	4,4,4	0.31	0	6,6,6	0.45	0
5	SO4	L	403	-	4,4,4	0.29	0	6,6,6	0.16	0
5	SO4	E	203	-	4,4,4	0.21	0	6,6,6	0.30	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.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	202	SO4	1	0
5	F	413	SO4	2	0
5	L	407	SO4	1	0
5	I	405	SO4	1	0
5	H	206	SO4	1	0
5	C	405	SO4	1	0
5	C	404	SO4	1	0
5	L	409	SO4	1	0
5	E	202	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	68/88 (77%)	-0.32	0 100 100	59, 78, 98, 102	0
1	D	65/88 (73%)	-0.08	1 (1%) 72 63	64, 85, 100, 119	0
1	G	67/88 (76%)	-0.35	1 (1%) 72 63	60, 75, 93, 97	0
1	J	66/88 (75%)	0.08	2 (3%) 52 42	72, 98, 119, 124	0
2	B	165/187 (88%)	-0.50	2 (1%) 76 68	51, 68, 91, 115	0
2	E	165/187 (88%)	-0.34	1 (0%) 85 80	43, 74, 100, 117	1 (0%)
2	H	165/187 (88%)	-0.54	1 (0%) 85 80	52, 67, 91, 108	0
2	K	164/187 (87%)	-0.24	3 (1%) 67 58	58, 79, 104, 116	0
3	C	308/321 (95%)	-0.65	4 (1%) 75 66	50, 63, 81, 112	0
3	F	308/321 (95%)	-0.57	1 (0%) 90 86	53, 66, 87, 121	0
3	I	309/321 (96%)	-0.65	2 (0%) 85 80	51, 62, 81, 115	1 (0%)
3	L	306/321 (95%)	-0.53	1 (0%) 90 86	57, 70, 90, 113	0
All	All	2156/2384 (90%)	-0.49	19 (0%) 81 74	43, 68, 99, 124	2 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	25[A]	PHE	7.3
2	B	182	LEU	5.3
1	D	86	LEU	4.8
1	J	86	LEU	4.1
2	H	182	LEU	4.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
5	SO4	C	409	5/5	0.67	0.15	64,73,79,82	1
5	SO4	I	406	5/5	0.71	0.10	65,76,79,80	1
5	SO4	K	207	5/5	0.71	0.10	96,104,108,109	2
5	SO4	B	206	5/5	0.73	0.12	91,98,101,104	1
5	SO4	K	205	5/5	0.77	0.10	77,83,87,89	1
5	SO4	K	202	5/5	0.78	0.11	69,79,80,85	1
5	SO4	K	203	5/5	0.78	0.17	58,73,76,85	1
5	SO4	I	404	5/5	0.79	0.09	67,69,77,85	1
5	SO4	C	408	5/5	0.80	0.10	65,68,72,76	1
5	SO4	E	204	5/5	0.80	0.12	91,93,102,102	2
5	SO4	C	406	5/5	0.81	0.09	73,74,78,78	1
5	SO4	K	204	5/5	0.81	0.11	73,80,82,87	1
5	SO4	F	410	5/5	0.82	0.12	91,94,97,100	1
5	SO4	H	205	5/5	0.82	0.10	73,76,87,94	1
5	SO4	B	204	5/5	0.82	0.17	76,77,79,86	2
5	SO4	K	206	5/5	0.83	0.07	88,95,103,107	2
5	SO4	F	406	5/5	0.84	0.11	77,80,85,91	1
5	SO4	H	207	5/5	0.85	0.10	80,80,87,87	2
5	SO4	L	403	5/5	0.85	0.10	76,78,80,84	1
5	SO4	F	412	5/5	0.86	0.14	61,64,66,66	4
5	SO4	F	409	5/5	0.86	0.08	79,81,87,90	2
5	SO4	F	404	5/5	0.86	0.14	53,55,59,63	1
5	SO4	E	205	5/5	0.88	0.06	82,83,85,89	1
5	SO4	C	405	5/5	0.88	0.08	66,69,82,84	1
5	SO4	I	403	5/5	0.88	0.17	51,52,56,59	1
5	SO4	L	409	5/5	0.88	0.19	91,93,99,104	4
5	SO4	E	203	5/5	0.89	0.09	67,68,73,81	1
5	SO4	H	203	5/5	0.89	0.10	60,64,67,73	1
5	SO4	B	203	5/5	0.89	0.14	67,68,75,76	1
5	SO4	C	403	5/5	0.89	0.12	52,58,62,67	1
5	SO4	L	407	5/5	0.89	0.10	75,78,79,85	3
5	SO4	E	207	5/5	0.89	0.08	73,76,77,77	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	H	206	5/5	0.90	0.08	62,67,70,78	1
5	SO4	E	202	5/5	0.91	0.08	65,70,71,76	2
5	SO4	L	404	5/5	0.91	0.09	58,65,67,75	1
5	SO4	H	204	5/5	0.91	0.08	78,81,94,98	1
5	SO4	I	408	5/5	0.91	0.08	64,68,78,80	1
5	SO4	E	201	5/5	0.92	0.09	58,60,65,70	2
5	SO4	F	411	5/5	0.92	0.07	71,74,80,82	2
5	SO4	F	407	5/5	0.93	0.07	70,72,79,80	2
5	SO4	K	201	5/5	0.93	0.10	63,68,72,76	1
5	SO4	H	201	5/5	0.93	0.08	61,62,66,70	2
5	SO4	F	403	5/5	0.93	0.13	72,79,82,88	2
5	SO4	B	205	5/5	0.93	0.06	64,65,68,75	1
5	SO4	C	404	5/5	0.93	0.08	50,54,56,57	2
5	SO4	F	413	5/5	0.94	0.09	75,77,82,86	3
5	SO4	E	206	5/5	0.94	0.06	70,72,72,73	1
5	SO4	F	405	5/5	0.94	0.08	62,65,68,71	2
5	SO4	B	202	5/5	0.94	0.07	65,66,67,67	1
5	SO4	L	405	5/5	0.94	0.06	61,67,70,72	2
5	SO4	I	405	5/5	0.94	0.08	60,61,66,71	2
5	SO4	B	201	5/5	0.94	0.07	61,67,70,73	1
5	SO4	L	406	5/5	0.95	0.06	61,62,68,70	1
4	CA	J	101	1/1	0.95	0.07	102,102,102,102	0
5	SO4	L	408	5/5	0.95	0.05	68,78,81,85	1
5	SO4	H	202	5/5	0.95	0.08	54,61,62,63	1
4	CA	D	102	1/1	0.96	0.06	97,97,97,97	0
4	CA	J	102	1/1	0.96	0.05	110,110,110,110	0
5	SO4	C	407	5/5	0.96	0.06	59,62,67,68	2
5	SO4	F	408	5/5	0.97	0.04	58,58,61,68	1
4	CA	C	402	1/1	0.97	0.10	63,63,63,63	0
4	CA	A	101	1/1	0.97	0.06	81,81,81,81	0
4	CA	G	102	1/1	0.97	0.04	89,89,89,89	0
5	SO4	I	407	5/5	0.98	0.04	60,61,68,69	2
4	CA	G	101	1/1	0.98	0.08	72,72,72,72	0
4	CA	D	101	1/1	0.98	0.07	90,90,90,90	0
4	CA	I	401	1/1	0.98	0.07	62,62,62,62	0
4	CA	I	402	1/1	0.98	0.06	64,64,64,64	0
4	CA	A	102	1/1	0.98	0.04	86,86,86,86	0
4	CA	F	401	1/1	0.98	0.06	59,59,59,59	0
4	CA	L	402	1/1	0.98	0.06	72,72,72,72	0
4	CA	L	401	1/1	0.99	0.06	68,68,68,68	0
4	CA	C	401	1/1	0.99	0.06	64,64,64,64	0
4	CA	F	402	1/1	0.99	0.06	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.