W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 18, 2024 – 03:50 PM EST

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)

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

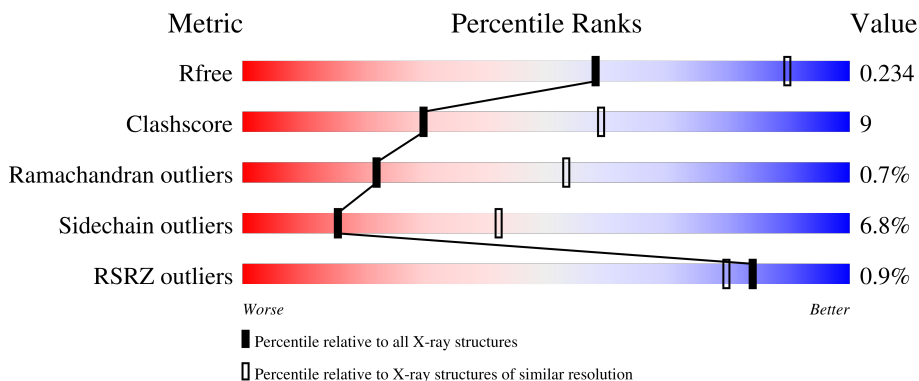|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.234
Clashscore		9
Ramachandran outliers		0.7%
Sidechain outliers		6.8%
RSRZ outliers		0.9%

Worse — *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	61% 13% • 23%
1	D	88	2% / 49% 23% • 26%
1	G	88	45% 25% 5% • 24%
1	J	88	3% / 39% 31% 6% 25%
2	B	187	% / 77% 11% • 12%

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Mol	Chain	Length	Quality of chain
2	E	187	61% 23% · 12%
2	H	187	72% 16% · 12%
2	K	187	67% 19% · 12%
3	C	321	73% 21% · ·
3	F	321	74% 19% · ·
3	I	321	74% 21% · ·
3	L	321	80% 14% · 5%

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 ⓘ

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 2260	C 1449	N 357	O 448	S 6	0	0	0
3	F	308	Total 2301	C 1471	N 363	O 461	S 6	0	0	0
3	I	309	Total 2290	C 1466	N 359	O 459	S 6	1	0	0
3	L	306	Total 2268	C 1451	N 354	O 457	S 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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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	A	2	Total 2	Ca 2	0	0
4	C	2	Total 2	Ca 2	0	0
4	D	2	Total 2	Ca 2	0	0
4	F	2	Total 2	Ca 2	0	0
4	G	2	Total 2	Ca 2	0	0
4	I	2	Total 2	Ca 2	0	0
4	J	2	Total 2	Ca 2	0	0
4	L	2	Total 2	Ca 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3 O⁻ — S — O⁻ O4

S

O2
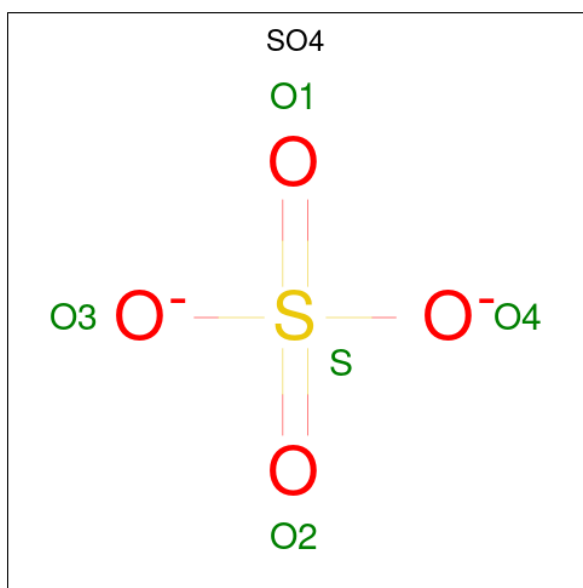
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	1	0
5	B	1	Total 5	O 4	S 1	1	0
5	B	1	Total 5	O 4	S 1	1	0
5	B	1	Total 5	O 4	S 1	0	0
5	C	1	Total 5	O 4	S 1	0	0
5	C	1	Total 5	O 4	S 1	1	0
5	C	1	Total 5	O 4	S 1	1	0
5	C	1	Total 5	O 4	S 1	1	0
5	C	1	Total 5	O 4	S 1	0	0
5	C	1	Total 5	O 4	S 1	1	0
5	C	1	Total 5	O 4	S 1	1	0

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

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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 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	0	0

- Molecule 6 is water.

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

3 Residue-property plots ⓘ

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.
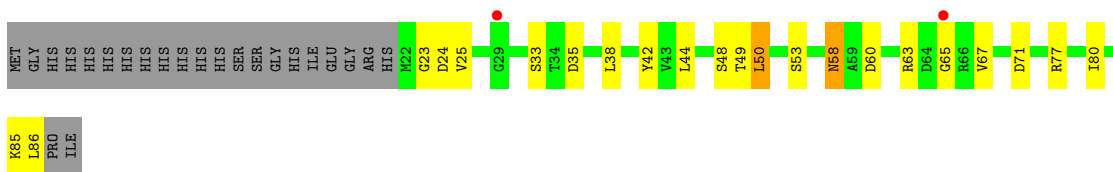
- Molecule 1: Glycoside hydrolase family 9

Chain A:
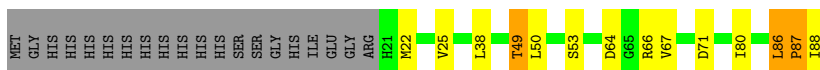
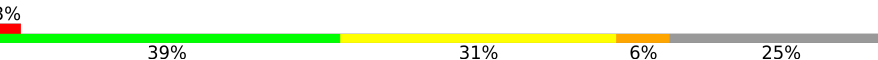- Molecule 1: Glycoside hydrolase family 9

Chain D:

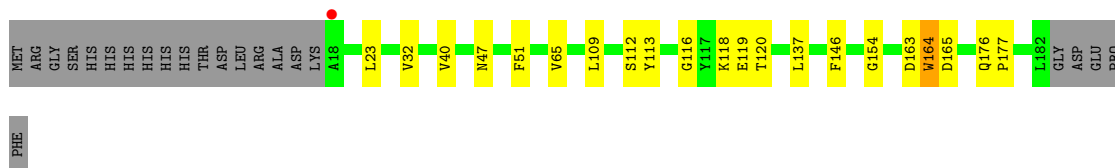- Molecule 1: Glycoside hydrolase family 9

Chain G:

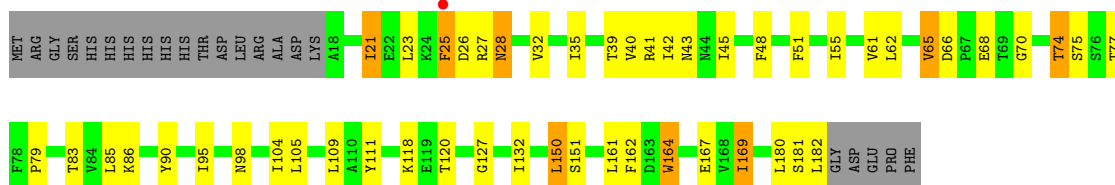- Molecule 1: Glycoside hydrolase family 9

Chain J:
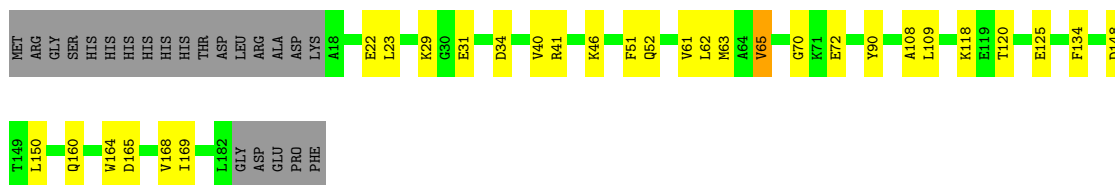
- Molecule 2: Scaffolding dockerin binding protein A

Chain B:

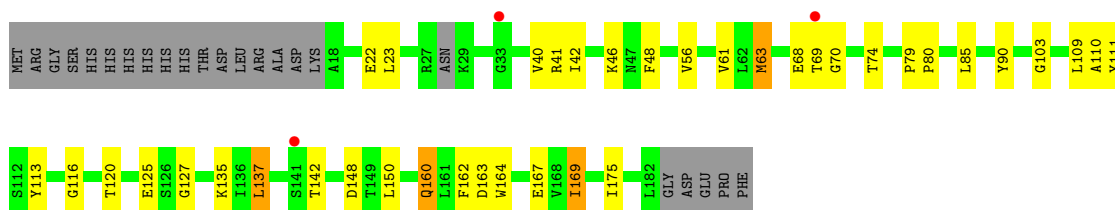MET ARG GLY SER HIS HIS HIS HIS HIS THR ASP LEU ARG ALA ASP LYS A18 L23 V32 V40 N47 F51 V65 L109 S112 Y113 G116 Y117 K118 E119 T120 L137 F146 G154 D163 W164 D165 Q176 P177 L182 GLY ASP GLU PRO

PHE

• Molecule 2: Scaffolding dockerin binding protein A

Chain E:

MET ARG GLY SER HIS HIS HIS HIS HIS THR ASP LEU ARG ALA ASP LYS A18 I21 E22 L23 K24 F25 D26 R27 N28 V32 I35 T39 V40 R41 I42 N43 N44 I45 F48 F51 I55 V61 L62 V65 D66 P67 E68 T69 G70 T74 S75 S76 T77

F78 P79 T83 V84 L85 K86 Y90 I95 N98 I104 L105 L109 Y111 K118 E119 T120 G127 I132 L150 S151 L161 F162 D163 W164 E167 V168 I169 L180 S181 L182 GLY ASP GLU PRO PHE

• Molecule 2: Scaffolding dockerin binding protein A

Chain H:

MET ARG GLY SER HIS HIS HIS HIS HIS THR ASP LEU ARG ALA ASP LYS A18 E22 L23 K29 G30 E31 D34 V40 R41 K46 F51 Q52 V61 L62 M63 A64 V65 G70 K71 E72 Y90 A108 L109 K118 E119 T120 E125 F134 D148

T149 L150 Q160 W164 D165 V168 I169 L182 GLY ASP GLU PRO PHE
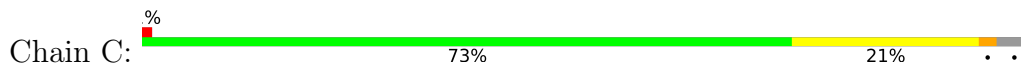
• Molecule 2: Scaffolding dockerin binding protein A

Chain K:

MET ARG GLY SER HIS HIS HIS HIS HIS THR ASP LEU ARG ALA ASP LYS A18 E22 L23 R27 ASN K29 G33 V40 R41 I42 K46 N47 F48 V56 V61 L62 M63 E68 T69 G70 T74 P79 P80 L85 Y90 G103 L109 A110 Y111

S112 Y113 G116 T120 E125 S126 G127 K135 I136 L137 S141 T142 D148 T149 L150 Q160 L161 F162 D163 W164 E167 V168 I169 I175 L182 GLY ASP GLU PRO PHE

• Molecule 3: Cellulosome anchoring protein cohesin region

Chain C:

MET PRO THR ILE THR P6 N7 K8 L9 G14 R15 R19 P27 G37 G41 P49 I57 T74 A75 V76 Y77 P78 D79 R80 K81 E89 Y96 A115 P116 E117 G118 A129 D132 L135 T140 V149 T150 P153 V154 I155 E156 G157 Y158

Y163 I164 L165 P166 D167 F168 A172 T173 V174 A175 V178 T189 E190 L191 Y200 F201 E202 V206 G212 L215 K216 I217 S218 R219 V230 V231 G234 S237 T240 M246 G250 D251 I252 V253 K254 D255 N256 E265 T273 S276 A277 N278 Y279

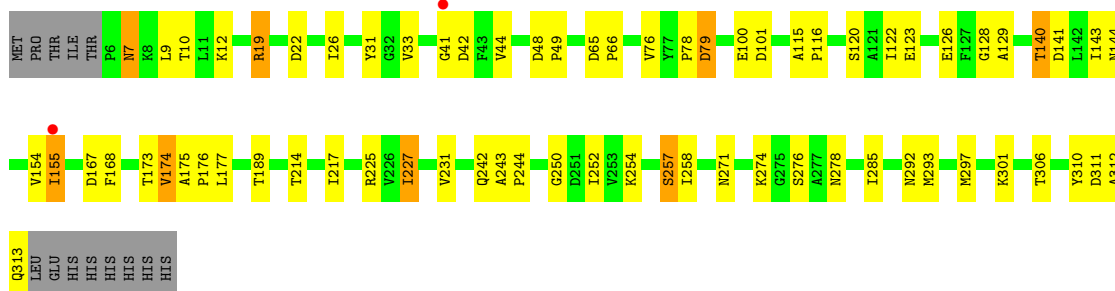V280 I285 N286 R287 I298 K301 T306 S307 S308 D309 Y310 D311 A312 Q313 LEU GLU HIS HIS HIS HIS HIS HIS
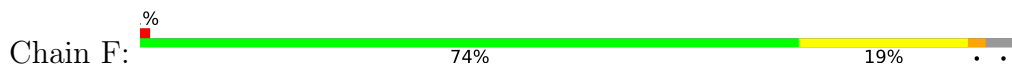
• Molecule 3: Cellulosome anchoring protein cohesin region

Chain F:

• Molecule 3: Cellulosome anchoring protein cohesin region

Chain I:

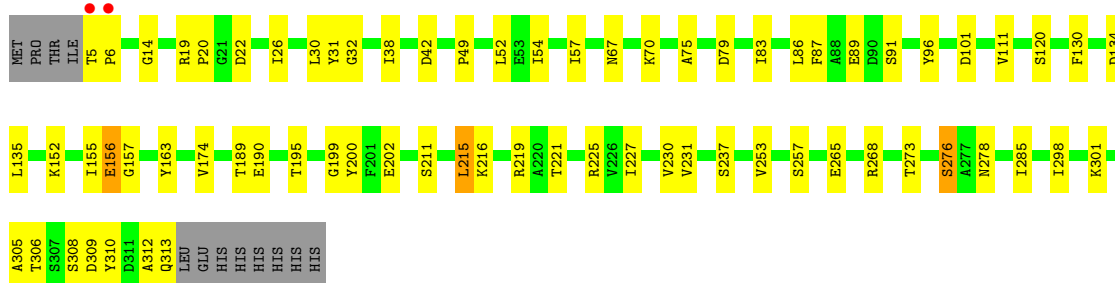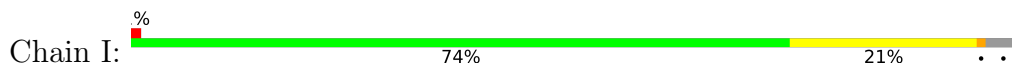• Molecule 3: Cellulosome anchoring protein cohesin region

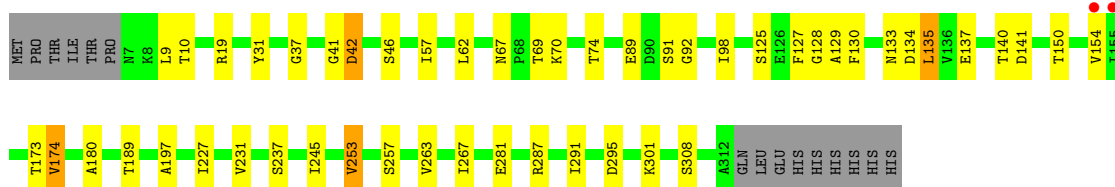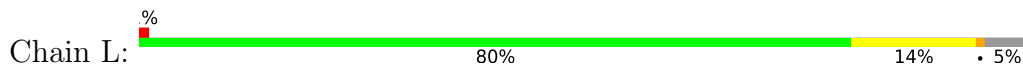Chain L:

4 Data and refinement statistics ⓘ

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) 99.5 (19.95-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.191 , 0.236 0.187 , 0.234	Depositor DCC
R_{free} test set	5224 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.4	EDS
L-test for twinning [2]	$< \lvert L \rvert > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
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

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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA

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 ⓘ

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%)	4	15
1	D	63/88 (72%)	54 (86%)	9 (14%)	0	100	100
1	G	65/88 (74%)	60 (92%)	4 (6%)	1 (2%)	10	33
1	J	64/88 (73%)	54 (84%)	8 (12%)	2 (3%)	4	14
2	B	163/187 (87%)	156 (96%)	6 (4%)	1 (1%)	25	56
2	E	164/187 (88%)	158 (96%)	5 (3%)	1 (1%)	25	56
2	H	163/187 (87%)	158 (97%)	5 (3%)	0	100	100
2	K	160/187 (86%)	147 (92%)	12 (8%)	1 (1%)	25	56
3	C	306/321 (95%)	286 (94%)	19 (6%)	1 (0%)	41	72
3	F	306/321 (95%)	289 (94%)	15 (5%)	2 (1%)	22	53
3	I	307/321 (96%)	284 (92%)	19 (6%)	4 (1%)	12	36
3	L	304/321 (95%)	282 (93%)	22 (7%)	0	100	100
All	All	2131/2384 (89%)	1986 (93%)	130 (6%)	15 (1%)	22	53

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%)	8	26
1	D	51/79 (65%)	46 (90%)	5 (10%)	8	24
1	G	56/79 (71%)	49 (88%)	7 (12%)	4	14
1	J	53/79 (67%)	49 (92%)	4 (8%)	13	37
2	B	126/156 (81%)	122 (97%)	4 (3%)	39	73
2	E	124/156 (80%)	109 (88%)	15 (12%)	5	15
2	H	129/156 (83%)	121 (94%)	8 (6%)	18	47
2	K	123/156 (79%)	114 (93%)	9 (7%)	14	38
3	C	233/266 (88%)	218 (94%)	15 (6%)	17	45
3	F	246/266 (92%)	231 (94%)	15 (6%)	18	48
3	I	241/266 (91%)	226 (94%)	15 (6%)	18	47
3	L	240/266 (90%)	228 (95%)	12 (5%)	24	56
All	All	1675/2004 (84%)	1561 (93%)	114 (7%)	16	42

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

Mol	Chain	Res	Type
3	F	257	SER
3	L	231	VAL
2	H	164	TRP
3	L	189	THR
2	K	160	GLN

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

Mol	Chain	Res	Type
3	I	313	GLN
1	J	21	HIS
1	J	68	ASN
2	E	28	ASN
3	C	278	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	F	412	-	4,4,4	0.20	0	6,6,6	0.57	0
5	SO4	I	404	-	4,4,4	0.15	0	6,6,6	0.23	0
5	SO4	I	407	-	4,4,4	0.16	0	6,6,6	0.28	0
5	SO4	B	206	-	4,4,4	0.11	0	6,6,6	0.28	0
5	SO4	I	406	-	4,4,4	0.08	0	6,6,6	0.46	0
5	SO4	L	405	-	4,4,4	0.11	0	6,6,6	0.29	0
5	SO4	H	207	-	4,4,4	0.20	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	SO4	E	202	-	4,4,4	0.13	0	6,6,6	0.28	0
5	SO4	F	405	-	4,4,4	0.14	0	6,6,6	0.24	0
5	SO4	C	406	-	4,4,4	0.14	0	6,6,6	0.19	0
5	SO4	K	202	-	4,4,4	0.15	0	6,6,6	0.33	0
5	SO4	F	411	-	4,4,4	0.13	0	6,6,6	0.13	0
5	SO4	C	405	-	4,4,4	0.18	0	6,6,6	0.31	0
5	SO4	B	202	-	4,4,4	0.12	0	6,6,6	0.28	0
5	SO4	F	410	-	4,4,4	0.14	0	6,6,6	0.22	0
5	SO4	L	403	-	4,4,4	0.19	0	6,6,6	0.22	0
5	SO4	E	207	-	4,4,4	0.19	0	6,6,6	0.17	0
5	SO4	F	403	-	4,4,4	0.15	0	6,6,6	0.20	0
5	SO4	H	201	-	4,4,4	0.21	0	6,6,6	0.36	0
5	SO4	K	206	-	4,4,4	0.10	0	6,6,6	0.23	0
5	SO4	F	408	-	4,4,4	0.16	0	6,6,6	0.09	0
5	SO4	L	409	-	4,4,4	0.20	0	6,6,6	0.19	0
5	SO4	E	206	-	4,4,4	0.20	0	6,6,6	0.48	0
5	SO4	F	404	-	4,4,4	0.27	0	6,6,6	0.77	0
5	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.36	0
5	SO4	E	205	-	4,4,4	0.18	0	6,6,6	0.49	0
5	SO4	L	404	-	4,4,4	0.16	0	6,6,6	0.37	0
5	SO4	C	408	-	4,4,4	0.15	0	6,6,6	0.24	0
5	SO4	H	205	-	4,4,4	0.22	0	6,6,6	0.32	0
5	SO4	K	201	-	4,4,4	0.15	0	6,6,6	0.32	0
5	SO4	B	203	-	4,4,4	0.20	0	6,6,6	0.29	0
5	SO4	E	201	-	4,4,4	0.16	0	6,6,6	0.37	0
5	SO4	I	408	-	4,4,4	0.15	0	6,6,6	0.29	0
5	SO4	L	406	-	4,4,4	0.17	0	6,6,6	0.43	0
5	SO4	H	202	-	4,4,4	0.24	0	6,6,6	0.88	0
5	SO4	F	409	-	4,4,4	0.20	0	6,6,6	0.25	0
5	SO4	K	207	-	4,4,4	0.16	0	6,6,6	0.18	0
5	SO4	B	205	-	4,4,4	0.14	0	6,6,6	0.28	0
5	SO4	C	409	-	4,4,4	0.12	0	6,6,6	0.59	0
5	SO4	K	205	-	4,4,4	0.22	0	6,6,6	0.30	0
5	SO4	B	204	-	4,4,4	0.14	0	6,6,6	0.40	0
5	SO4	H	203	-	4,4,4	0.16	0	6,6,6	0.23	0
5	SO4	H	206	-	4,4,4	0.17	0	6,6,6	0.31	0
5	SO4	I	405	-	4,4,4	0.15	0	6,6,6	0.14	0
5	SO4	L	407	-	4,4,4	0.14	0	6,6,6	0.22	0
5	SO4	H	204	-	4,4,4	0.13	0	6,6,6	0.17	0
5	SO4	C	403	-	4,4,4	0.24	0	6,6,6	0.57	0
5	SO4	B	201	-	4,4,4	0.17	0	6,6,6	0.66	0
5	SO4	F	413	-	4,4,4	0.14	0	6,6,6	0.18	0
5	SO4	K	203	-	4,4,4	0.25	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	SO4	F	407	-	4,4,4	0.17	0	6,6,6	0.28	0
5	SO4	E	203	-	4,4,4	0.12	0	6,6,6	0.31	0
5	SO4	F	406	-	4,4,4	0.18	0	6,6,6	0.22	0
5	SO4	I	403	-	4,4,4	0.28	0	6,6,6	0.66	0
5	SO4	K	204	-	4,4,4	0.19	0	6,6,6	0.23	0
5	SO4	E	204	-	4,4,4	0.13	0	6,6,6	0.18	0
5	SO4	C	407	-	4,4,4	0.16	0	6,6,6	0.23	0
5	SO4	L	408	-	4,4,4	0.18	0	6,6,6	0.19	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	E	202	SO4	1	0
5	C	405	SO4	1	0
5	L	409	SO4	1	0
5	C	404	SO4	1	0
5	H	202	SO4	1	0
5	I	405	SO4	1	0
5	L	407	SO4	1	0
5	F	413	SO4	2	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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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, 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%)	-0.25	0	100	100	59, 78, 98, 102	0
1	D	65/88 (73%)	-0.13	2 (3%)	49	39	64, 85, 100, 119	0
1	G	67/88 (76%)	-0.21	0	100	100	60, 75, 93, 97	0
1	J	66/88 (75%)	0.08	3 (4%)	33	23	72, 98, 119, 124	0
2	B	165/187 (88%)	-0.39	1 (0%)	89	86	51, 68, 91, 115	0
2	E	165/187 (88%)	-0.31	1 (0%)	89	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%)	-0.22	3 (1%)	68	61	58, 79, 104, 116	0
3	C	308/321 (95%)	-0.48	3 (0%)	82	77	50, 63, 81, 112	0
3	F	308/321 (95%)	-0.37	2 (0%)	89	86	53, 66, 87, 121	0
3	I	309/321 (96%)	-0.47	2 (0%)	89	86	51, 62, 81, 115	1 (0%)
3	L	306/321 (95%)	-0.39	2 (0%)	87	84	57, 70, 90, 113	0
All	All	2156/2384 (90%)	-0.36	19 (0%)	84	80	50, 69, 99, 124	1 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	69	THR	3.5
3	I	5	THR	3.4
1	J	21	HIS	2.9
3	C	153	PRO	2.8
1	D	29	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.

WORLDWIDE PDB
PROTEIN DATA BANK

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	K	203	5/5	0.66	0.39	58,73,76,85	1
5	SO4	F	410	5/5	0.70	0.29	91,94,97,100	1
5	SO4	C	409	5/5	0.72	0.28	64,73,79,82	1
5	SO4	F	407	5/5	0.79	0.30	70,72,79,80	2
5	SO4	B	204	5/5	0.80	0.50	76,77,79,86	2
5	SO4	I	406	5/5	0.82	0.18	65,76,79,80	1
5	SO4	K	205	5/5	0.82	0.26	77,83,87,89	1
5	SO4	F	412	5/5	0.83	0.47	61,64,66,66	4
5	SO4	K	202	5/5	0.83	0.26	69,79,80,85	1
5	SO4	K	204	5/5	0.84	0.39	73,80,82,87	1
5	SO4	C	406	5/5	0.84	0.31	73,74,78,78	1
5	SO4	F	406	5/5	0.85	0.28	77,80,85,91	1
5	SO4	I	408	5/5	0.85	0.25	64,68,78,80	1
5	SO4	F	413	5/5	0.85	0.34	75,77,82,86	3
5	SO4	L	403	5/5	0.86	0.28	76,78,80,84	1
5	SO4	B	205	5/5	0.87	0.25	64,65,68,75	1
5	SO4	E	202	5/5	0.87	0.29	65,70,71,76	2
5	SO4	H	204	5/5	0.88	0.24	78,81,94,98	1
5	SO4	F	411	5/5	0.88	0.25	71,74,80,82	2
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	H	205	5/5	0.89	0.27	73,76,87,94	1
5	SO4	C	408	5/5	0.89	0.22	65,68,72,76	1
5	SO4	F	404	5/5	0.90	0.17	53,55,59,63	1
5	SO4	C	405	5/5	0.90	0.23	66,69,82,84	1
5	SO4	L	408	5/5	0.90	0.23	68,78,81,85	1
4	CA	A	102	1/1	0.91	0.10	86,86,86,86	0
5	SO4	I	404	5/5	0.91	0.24	67,69,77,85	1
5	SO4	B	206	5/5	0.91	0.14	91,98,101,104	1
5	SO4	F	409	5/5	0.91	0.24	79,81,87,90	2
5	SO4	F	405	5/5	0.91	0.24	62,65,68,71	2
5	SO4	H	201	5/5	0.92	0.25	61,62,66,70	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	I	405	5/5	0.92	0.25	60,61,66,71	2
5	SO4	H	203	5/5	0.92	0.14	60,64,67,73	1
5	SO4	B	203	5/5	0.92	0.18	67,68,75,76	1
5	SO4	E	206	5/5	0.92	0.30	70,72,72,73	1
5	SO4	H	206	5/5	0.93	0.30	62,67,70,78	1
5	SO4	H	207	5/5	0.93	0.16	80,80,87,87	2
5	SO4	H	202	5/5	0.93	0.13	54,61,62,63	1
4	CA	C	402	1/1	0.93	0.25	63,63,63,63	0
5	SO4	K	206	5/5	0.93	0.15	88,95,103,107	2
4	CA	D	102	1/1	0.93	0.09	97,97,97,97	0
5	SO4	L	407	5/5	0.93	0.35	75,78,79,85	3
5	SO4	E	205	5/5	0.93	0.33	82,83,85,89	1
5	SO4	L	409	5/5	0.93	0.45	91,93,99,104	4
5	SO4	I	403	5/5	0.94	0.20	51,52,56,59	1
5	SO4	C	403	5/5	0.94	0.14	52,58,62,67	1
4	CA	D	101	1/1	0.95	0.10	90,90,90,90	0
5	SO4	L	404	5/5	0.95	0.12	58,65,67,75	1
5	SO4	L	406	5/5	0.95	0.19	61,62,68,70	1
5	SO4	E	203	5/5	0.95	0.16	67,68,73,81	1
4	CA	G	102	1/1	0.95	0.09	89,89,89,89	0
5	SO4	B	201	5/5	0.95	0.13	61,67,70,73	1
5	SO4	K	207	5/5	0.96	0.32	96,104,108,109	2
4	CA	G	101	1/1	0.96	0.15	72,72,72,72	0
5	SO4	B	202	5/5	0.96	0.13	65,66,67,67	1
4	CA	F	402	1/1	0.96	0.13	69,69,69,69	0
5	SO4	E	201	5/5	0.96	0.13	58,60,65,70	2
5	SO4	C	404	5/5	0.96	0.21	50,54,56,57	2
4	CA	J	102	1/1	0.96	0.10	110,110,110,110	0
4	CA	I	401	1/1	0.97	0.22	62,62,62,62	0
5	SO4	L	405	5/5	0.97	0.13	61,67,70,72	2
4	CA	J	101	1/1	0.97	0.13	102,102,102,102	0
5	SO4	K	201	5/5	0.97	0.11	63,68,72,76	1
4	CA	C	401	1/1	0.97	0.16	64,64,64,64	0
5	SO4	E	207	5/5	0.97	0.32	73,76,77,77	1
4	CA	L	402	1/1	0.98	0.13	72,72,72,72	0
4	CA	A	101	1/1	0.98	0.13	81,81,81,81	0
5	SO4	C	407	5/5	0.98	0.21	59,62,67,68	2
4	CA	I	402	1/1	0.98	0.15	64,64,64,64	0
5	SO4	I	407	5/5	0.99	0.10	60,61,68,69	2
4	CA	L	401	1/1	0.99	0.22	68,68,68,68	0
5	SO4	F	408	5/5	0.99	0.14	58,58,61,68	1
4	CA	F	401	1/1	0.99	0.21	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.