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 1, 2016 – 12:21 PM GMT

PDB ID	:	3QS3
Title	:	Crystal structure of the biofilm forming subunit of the E. coli common pilus: donor strand complemented (DSC) EcpA
Authors	:	Garnett, J.A.; Matthews, S.J.
Deposited on	:	2011-02-19
Resolution	:	2.10 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	:	1.7 (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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.
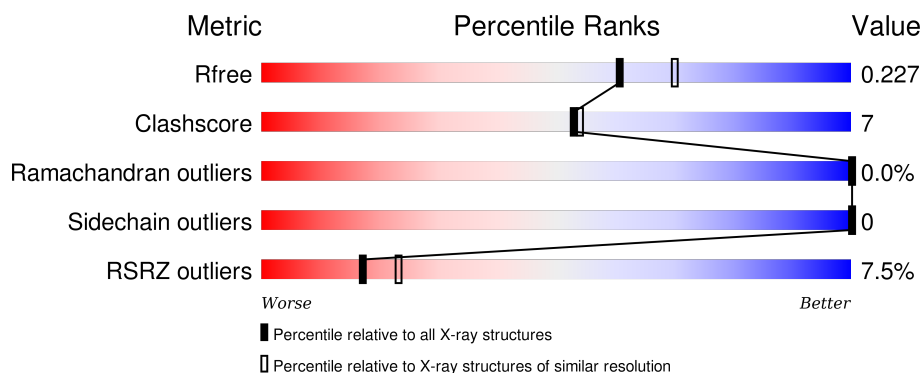
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 >=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 <=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	191	
1	B	191	
1	C	191	
1	D	191	
1	E	191	

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Mol	Chain	Length	Quality of chain
1	F	191	10% 82% 9% 8%
1	G	191	8% 86% 6% 8%
1	H	191	6% 88% • 7%
1	I	191	11% 78% 14% 8%
1	J	191	7% 81% 8% 11%
1	K	191	9% 82% 10% 8%
1	L	191	10% 87% 5% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	B	195	-	-	X	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16287 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 Fimbrillin matB homolog, EcpD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	4	0
			1279	802	207	269	1			
1	B	176	Total	C	N	O	S	0	3	0
			1293	807	212	273	1			
1	C	175	Total	C	N	O	S	0	1	0
			1272	793	207	271	1			
1	D	176	Total	C	N	O	S	0	3	0
			1292	805	213	273	1			
1	E	176	Total	C	N	O	S	0	0	0
			1268	789	211	267	1			
1	F	175	Total	C	N	O	S	0	3	0
			1285	801	212	271	1			
1	G	176	Total	C	N	O	S	0	4	0
			1284	802	207	274	1			
1	H	177	Total	C	N	O	S	0	2	0
			1278	794	209	274	1			
1	I	175	Total	C	N	O	S	0	2	0
			1268	790	207	270	1			
1	J	170	Total	C	N	O	S	0	1	0
			1236	774	204	257	1			
1	K	176	Total	C	N	O	S	0	1	0
			1273	794	209	269	1			
1	L	176	Total	C	N	O	S	0	1	0
			1257	784	208	264	1			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
A	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
A	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
A	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
A	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
A	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
A	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
A	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
A	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
A	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
A	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
A	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
A	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
A	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
A	174	SER	-	LINKER	UNP Q8CWB9
A	175	ASP	-	LINKER	UNP Q8CWB9
A	176	ASN	-	LINKER	UNP Q8CWB9
A	177	LYS	-	LINKER	UNP Q8CWB9
B	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
B	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
B	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
B	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
B	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
B	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
B	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
B	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
B	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
B	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
B	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
B	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
B	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
B	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
B	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
B	174	SER	-	LINKER	UNP Q8CWB9
B	175	ASP	-	LINKER	UNP Q8CWB9
B	176	ASN	-	LINKER	UNP Q8CWB9
B	177	LYS	-	LINKER	UNP Q8CWB9
C	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
C	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
C	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
C	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
C	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
C	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
C	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
C	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
C	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
C	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
C	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
C	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
C	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
C	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
C	174	SER	-	LINKER	UNP Q8CWB9
C	175	ASP	-	LINKER	UNP Q8CWB9
C	176	ASN	-	LINKER	UNP Q8CWB9
C	177	LYS	-	LINKER	UNP Q8CWB9
D	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
D	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
D	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
D	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
D	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
D	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
D	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
D	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
D	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
D	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
D	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
D	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
D	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
D	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
D	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
D	174	SER	-	LINKER	UNP Q8CWB9
D	175	ASP	-	LINKER	UNP Q8CWB9
D	176	ASN	-	LINKER	UNP Q8CWB9
D	177	LYS	-	LINKER	UNP Q8CWB9
E	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
E	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
E	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
E	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
E	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
E	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
E	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
E	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
E	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
E	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
E	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
E	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
E	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
E	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
E	174	SER	-	LINKER	UNP Q8CWB9
E	175	ASP	-	LINKER	UNP Q8CWB9
E	176	ASN	-	LINKER	UNP Q8CWB9
E	177	LYS	-	LINKER	UNP Q8CWB9
F	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
F	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
F	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
F	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
F	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
F	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
F	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
F	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
F	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
F	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
F	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
F	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
F	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
F	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
F	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
F	174	SER	-	LINKER	UNP Q8CWB9
F	175	ASP	-	LINKER	UNP Q8CWB9
F	176	ASN	-	LINKER	UNP Q8CWB9
F	177	LYS	-	LINKER	UNP Q8CWB9
G	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
G	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
G	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
G	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
G	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
G	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
G	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
G	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
G	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
G	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
G	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
G	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
G	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
G	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
G	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
G	174	SER	-	LINKER	UNP Q8CWB9
G	175	ASP	-	LINKER	UNP Q8CWB9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	176	ASN	-	LINKER	UNP Q8CWB9
G	177	LYS	-	LINKER	UNP Q8CWB9
H	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
H	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
H	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
H	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
H	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
H	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
H	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
H	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
H	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
H	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
H	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
H	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
H	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
H	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
H	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
H	174	SER	-	LINKER	UNP Q8CWB9
H	175	ASP	-	LINKER	UNP Q8CWB9
H	176	ASN	-	LINKER	UNP Q8CWB9
H	177	LYS	-	LINKER	UNP Q8CWB9
I	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
I	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
I	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
I	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
I	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
I	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
I	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
I	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
I	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
I	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
I	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
I	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
I	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
I	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
I	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
I	174	SER	-	LINKER	UNP Q8CWB9
I	175	ASP	-	LINKER	UNP Q8CWB9
I	176	ASN	-	LINKER	UNP Q8CWB9
I	177	LYS	-	LINKER	UNP Q8CWB9
J	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
J	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
J	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
J	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
J	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
J	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
J	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
J	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
J	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
J	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
J	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
J	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
J	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
J	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
J	174	SER	-	LINKER	UNP Q8CWB9
J	175	ASP	-	LINKER	UNP Q8CWB9
J	176	ASN	-	LINKER	UNP Q8CWB9
J	177	LYS	-	LINKER	UNP Q8CWB9
K	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
K	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
K	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
K	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
K	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
K	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9
K	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
K	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
K	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
K	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
K	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
K	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
K	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
K	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
K	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
K	174	SER	-	LINKER	UNP Q8CWB9
K	175	ASP	-	LINKER	UNP Q8CWB9
K	176	ASN	-	LINKER	UNP Q8CWB9
K	177	LYS	-	LINKER	UNP Q8CWB9
L	4	MET	-	EXPRESSION TAG	UNP Q8CWB9
L	5	ALA	-	EXPRESSION TAG	UNP Q8CWB9
L	6	HIS	-	EXPRESSION TAG	UNP Q8CWB9
L	7	HIS	-	EXPRESSION TAG	UNP Q8CWB9
L	8	HIS	-	EXPRESSION TAG	UNP Q8CWB9
L	9	HIS	-	EXPRESSION TAG	UNP Q8CWB9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	10	HIS	-	EXPRESSION TAG	UNP Q8CWB9
L	11	HIS	-	EXPRESSION TAG	UNP Q8CWB9
L	12	VAL	-	EXPRESSION TAG	UNP Q8CWB9
L	13	ASP	-	EXPRESSION TAG	UNP Q8CWB9
L	14	ASP	-	EXPRESSION TAG	UNP Q8CWB9
L	15	ASP	-	EXPRESSION TAG	UNP Q8CWB9
L	16	ASP	-	EXPRESSION TAG	UNP Q8CWB9
L	17	LYS	-	EXPRESSION TAG	UNP Q8CWB9
L	18	MET	-	EXPRESSION TAG	UNP Q8CWB9
L	174	SER	-	LINKER	UNP Q8CWB9
L	175	ASP	-	LINKER	UNP Q8CWB9
L	176	ASN	-	LINKER	UNP Q8CWB9
L	177	LYS	-	LINKER	UNP Q8CWB9

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).
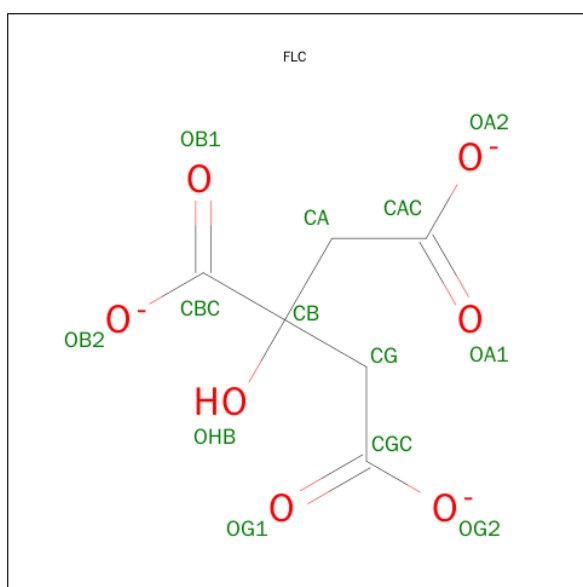
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 13	C 6	O 7	0	0
2	D	1	Total 13	C 6	O 7	0	0
2	F	1	Total 13	C 6	O 7	0	0
2	G	1	Total 13	C 6	O 7	0	0
2	I	1	Total 13	C 6	O 7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total 13	C 6	O 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	0	0
3	B	104	Total 104	O 104	0	0
3	C	108	Total 108	O 108	0	0
3	D	96	Total 96	O 96	0	0
3	E	69	Total 69	O 69	0	0
3	F	90	Total 90	O 90	0	0
3	G	87	Total 87	O 87	0	0
3	H	71	Total 71	O 71	0	0
3	I	77	Total 77	O 77	0	0
3	J	35	Total 35	O 35	0	0
3	K	72	Total 72	O 72	0	0
3	L	47	Total 47	O 47	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
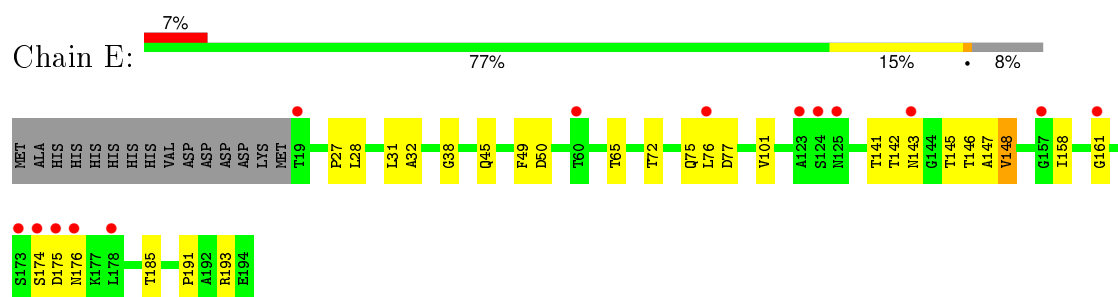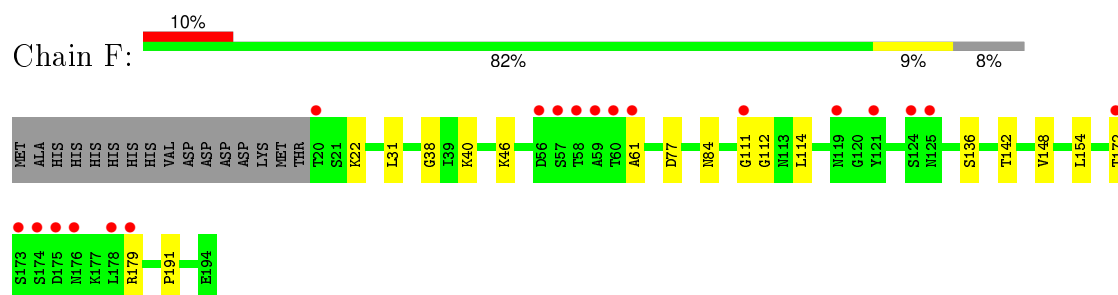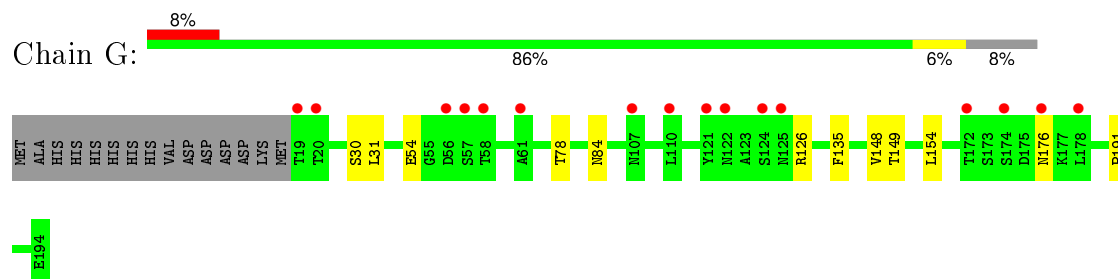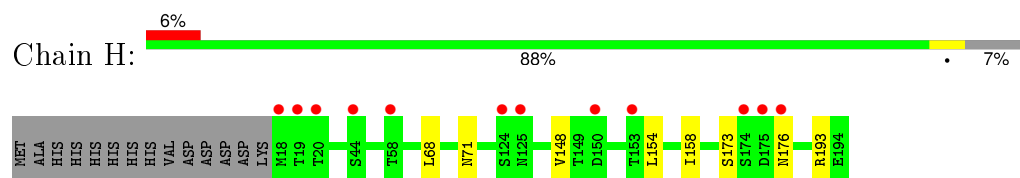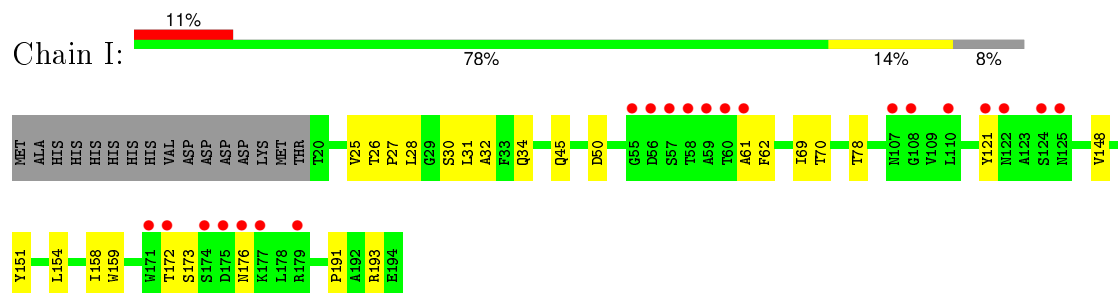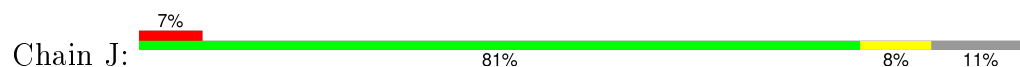
- Molecule 1: Fimbrillin matB homolog, EcpD
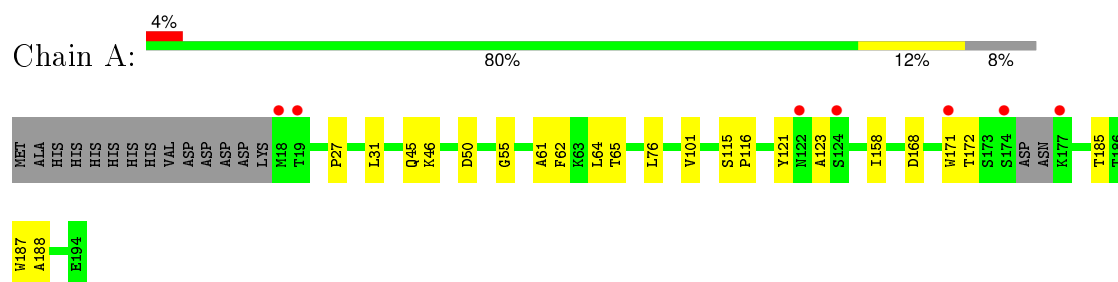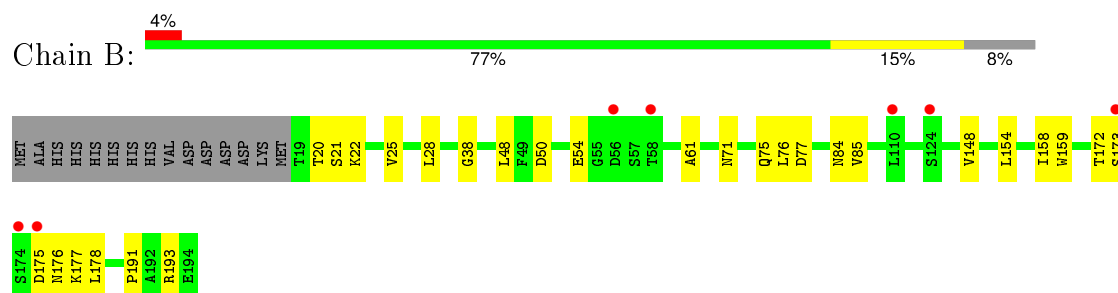
- Molecule 1: Fimbrillin matB homolog, EcpD

- Molecule 1: Fimbrillin matB homolog, EcpD

- Molecule 1: Fimbrillin matB homolog, EcpD

- Molecule 1: Fimbrillin matB homolog, EcpD

Chain E:

Chain E residue plot

• Molecule 1: Fimbrillin matB homolog, EcpD

Chain F:

Chain F residue plot

• Molecule 1: Fimbrillin matB homolog, EcpD

Chain G:

Chain G residue plot

• Molecule 1: Fimbrillin matB homolog, EcpD

Chain H:

Chain H residue plot

• Molecule 1: Fimbrillin matB homolog, EcpD
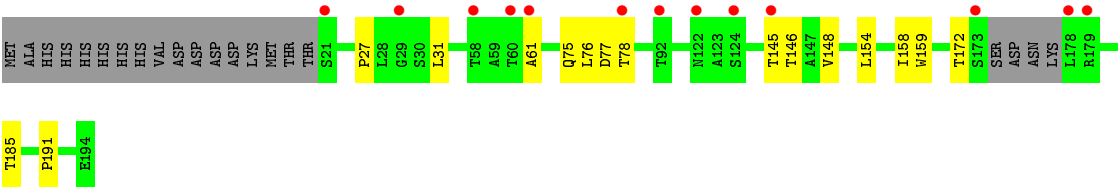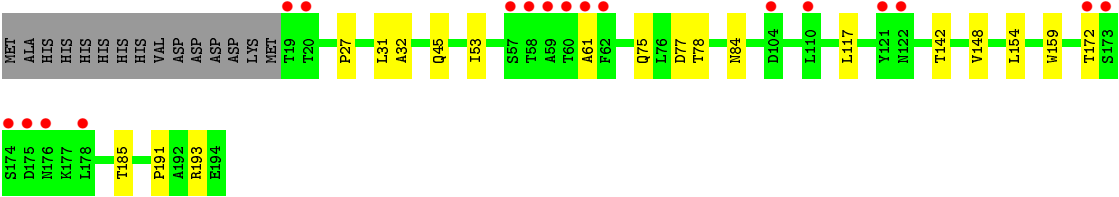
Chain I:

Chain I residue plot

• Molecule 1: Fimbrillin matB homolog, EcpD

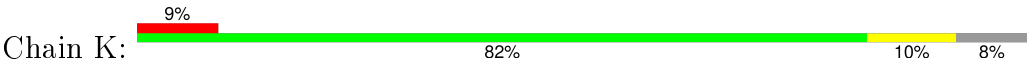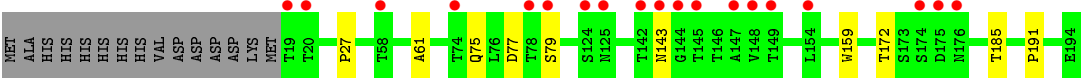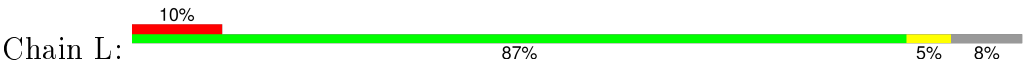Chain J:

• Molecule 1: Fimbrillin matB homolog, EcpD

Chain K:

• Molecule 1: Fimbrillin matB homolog, EcpD

Chain L:
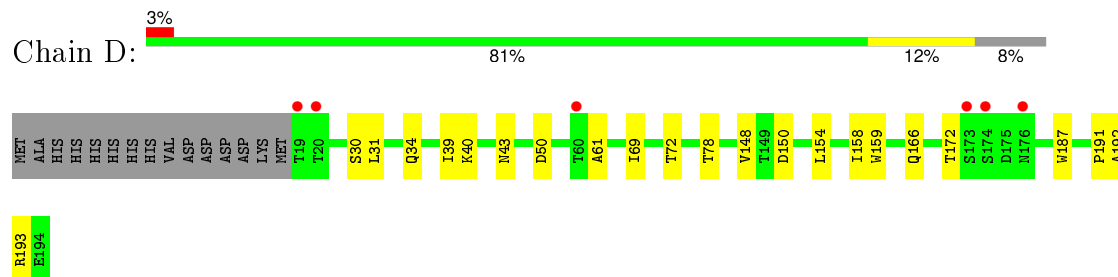
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	101.79Å 101.79Å 387.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.17 – 2.10 50.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (88.17-2.10) 98.6 (50.90-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.42	Depositor
$<I/\sigma(I)>$ [1]	3.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.167 , 0.200 0.194 , 0.227	Depositor DCC
R_{free} test set	12887 reflections (11.03%)	DCC
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.6	EDS
Estimated twinning fraction	0.802 for H, K, L 0.198 for K, H, -L 0.012 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.802 for H, K, L 0.198 for K, H, -L	Depositor
L-test for twinning[2]	$<|L|> = 0.52, <L^2> = 0.36$	Xtriage
Outliers	0 of 129756 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16287	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 $<|L|>$, $<L^2>$ 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: FLC

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	0.71	0/1310	0.67	0/1791
1	B	0.55	0/1322	0.65	0/1806
1	C	0.66	0/1294	0.68	0/1767
1	D	0.63	0/1324	0.66	0/1810
1	E	0.63	0/1288	0.71	0/1760
1	F	0.55	0/1314	0.66	1/1795 (0.1%)
1	G	0.57	0/1316	0.64	0/1801
1	H	0.51	0/1306	0.65	0/1786
1	I	0.59	0/1294	0.63	0/1771
1	J	0.50	0/1258	0.63	0/1717
1	K	0.57	0/1296	0.65	0/1772
1	L	0.50	0/1280	0.63	0/1752
All	All	0.58	0/15602	0.66	1/21328 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	77	ASP	CB-CG-OD1	5.37	123.13	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	142	THR	Peptide

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	1279	0	1228	16	0
1	B	1293	0	1256	34	0
1	C	1272	0	1216	13	0
1	D	1292	0	1249	19	0
1	E	1268	0	1206	32	0
1	F	1285	0	1238	15	0
1	G	1284	0	1229	11	0
1	H	1278	0	1206	4	0
1	I	1268	0	1187	19	0
1	J	1236	0	1183	11	0
1	K	1273	0	1207	18	0
1	L	1257	0	1182	10	0
2	B	13	0	5	4	0
2	D	13	0	5	1	0
2	F	13	0	5	3	0
2	G	13	0	5	2	0
2	I	13	0	5	2	0
2	K	13	0	5	0	0
3	A	68	0	0	0	0
3	B	104	0	0	1	0
3	C	108	0	0	4	0
3	D	96	0	0	4	0
3	E	69	0	0	0	0
3	F	90	0	0	3	0
3	G	87	0	0	2	0
3	H	71	0	0	0	0
3	I	77	0	0	2	0
3	J	35	0	0	1	0
3	K	72	0	0	2	0
3	L	47	0	0	0	0
All	All	16287	0	14617	197	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 197 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:E:147:ALA:O	1:E:148:VAL:HG13	1.12	1.24
1:E:174:SER:HA	1:E:176:ASN:N	1.55	1.20
1:E:147:ALA:O	1:E:148:VAL:CG1	1.91	1.17
1:E:174:SER:CA	1:E:176:ASN:H	1.58	1.17
1:B:75:GLN:HG2	1:B:77:ASP:OD1	1.57	1.02

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	175/191 (92%)	165 (94%)	10 (6%)	0	100	100
1	B	177/191 (93%)	167 (94%)	10 (6%)	0	100	100
1	C	172/191 (90%)	165 (96%)	7 (4%)	0	100	100
1	D	178/191 (93%)	170 (96%)	8 (4%)	0	100	100
1	E	174/191 (91%)	162 (93%)	11 (6%)	1 (1%)	30	24
1	F	176/191 (92%)	166 (94%)	10 (6%)	0	100	100
1	G	178/191 (93%)	171 (96%)	7 (4%)	0	100	100
1	H	177/191 (93%)	169 (96%)	8 (4%)	0	100	100
1	I	175/191 (92%)	167 (95%)	8 (5%)	0	100	100
1	J	167/191 (87%)	160 (96%)	7 (4%)	0	100	100
1	K	175/191 (92%)	166 (95%)	9 (5%)	0	100	100
1	L	175/191 (92%)	166 (95%)	9 (5%)	0	100	100
All	All	2099/2292 (92%)	1994 (95%)	104 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	148	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	135/155 (87%)	135 (100%)	0	100	100
1	B	140/155 (90%)	140 (100%)	0	100	100
1	C	135/155 (87%)	135 (100%)	0	100	100
1	D	139/155 (90%)	139 (100%)	0	100	100
1	E	132/155 (85%)	132 (100%)	0	100	100
1	F	137/155 (88%)	137 (100%)	0	100	100
1	G	137/155 (88%)	137 (100%)	0	100	100
1	H	135/155 (87%)	135 (100%)	0	100	100
1	I	130/155 (84%)	130 (100%)	0	100	100
1	J	128/155 (83%)	128 (100%)	0	100	100
1	K	132/155 (85%)	132 (100%)	0	100	100
1	L	128/155 (83%)	128 (100%)	0	100	100
All	All	1608/1860 (86%)	1608 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	84	ASN
1	G	45	GLN
1	L	45	GLN
1	F	119	ASN
1	G	84	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	FLC	B	195	-	3,12,12	0.76	0	3,17,17	3.20	2 (66%)
2	FLC	D	1	-	3,12,12	1.29	0	3,17,17	4.43	2 (66%)
2	FLC	F	3	-	3,12,12	1.25	0	3,17,17	3.61	2 (66%)
2	FLC	G	2	-	3,12,12	0.71	0	3,17,17	5.30	3 (100%)
2	FLC	I	195	-	3,12,12	0.74	0	3,17,17	3.65	3 (100%)
2	FLC	K	195	-	3,12,12	0.84	0	3,17,17	2.83	2 (66%)

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
2	FLC	B	195	-	-	0/6/16/16	0/0/0/0
2	FLC	D	1	-	-	0/6/16/16	0/0/0/0
2	FLC	F	3	-	-	0/6/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	G	2	-	-	0/6/16/16	0/0/0/0
2	FLC	I	195	-	-	0/6/16/16	0/0/0/0
2	FLC	K	195	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	FLC	CB-CG-CGC	-6.85	104.01	114.96
2	D	1	FLC	CB-CA-CAC	-6.79	104.11	114.96
2	F	3	FLC	CB-CA-CAC	-5.60	106.00	114.96
2	I	195	FLC	CB-CG-CGC	-5.05	106.88	114.96
2	B	195	FLC	CB-CG-CGC	-3.62	109.17	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	195	FLC	4	0
2	D	1	FLC	1	0
2	F	3	FLC	3	0
2	G	2	FLC	2	0
2	I	195	FLC	2	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(Å²)	Q<0.9
1	A	175/191 (91%)	0.16	7 (4%)	42	51	18, 28, 46, 54	0
1	B	176/191 (92%)	0.29	7 (3%)	42	51	15, 25, 50, 64	0
1	C	175/191 (91%)	0.04	5 (2%)	55	63	18, 25, 42, 57	0
1	D	176/191 (92%)	0.18	6 (3%)	49	58	16, 26, 49, 67	0
1	E	176/191 (92%)	0.44	14 (7%)	15	21	18, 30, 58, 70	0
1	F	175/191 (91%)	0.43	19 (10%)	7	10	15, 26, 57, 72	0
1	G	176/191 (92%)	0.30	16 (9%)	11	16	17, 31, 62, 76	0
1	H	177/191 (92%)	0.27	12 (6%)	20	28	18, 30, 53, 65	1 (0%)
1	I	175/191 (91%)	0.50	21 (12%)	6	8	18, 30, 59, 79	0
1	J	170/191 (89%)	0.28	13 (7%)	17	23	22, 36, 53, 71	0
1	K	176/191 (92%)	0.45	18 (10%)	9	12	18, 32, 65, 85	0
1	L	176/191 (92%)	0.37	19 (10%)	8	10	19, 35, 70, 82	0
All	All	2103/2292 (91%)	0.31	157 (7%)	17	23	15, 30, 59, 85	1 (0%)

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	176	ASN	7.5
1	F	174	SER	7.4
1	K	176	ASN	7.0
1	I	174	SER	6.0
1	L	149	THR	6.0

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 carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	FLC	B	195	13/13	0.73	0.26	4.11	30,33,35,36	13
2	FLC	I	195	13/13	0.69	0.24	1.42	32,34,35,36	13
2	FLC	F	3	13/13	0.77	0.22	1.07	28,32,33,34	13
2	FLC	G	2	13/13	0.72	0.20	0.43	35,38,39,39	13
2	FLC	D	1	13/13	0.82	0.15	0.36	25,29,30,31	13
2	FLC	K	195	13/13	0.84	0.17	0.20	28,30,32,33	13

6.5 Other polymers (i)

There are no such residues in this entry.