Full wwPDB X-ray Structure Validation 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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

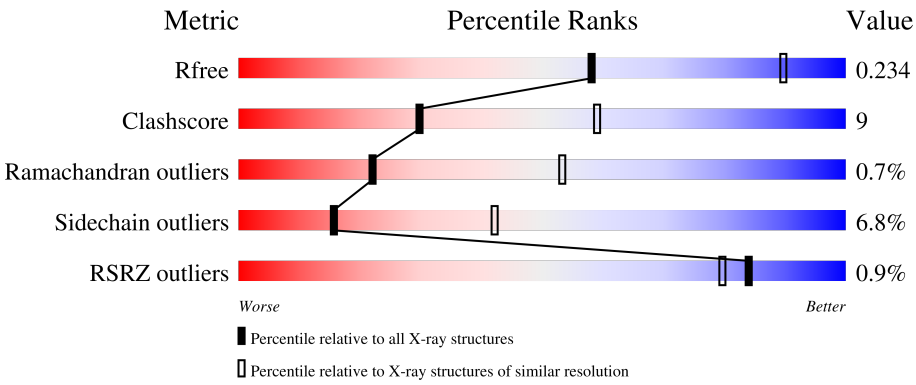
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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}	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 (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
			Total	C	N	O	S			
2	E	165	1223	788	194	239	2	0	1	0
			Total	C	N	O	S			
2	H	165	1237	797	194	244	2	0	0	0
			Total	C	N	O	S			
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
			Total	C	N	O	S			
3	F	308	2301	1471	363	461	6	0	0	0
			Total	C	N	O	S			
3	I	309	2290	1466	359	459	6	1	0	0
			Total	C	N	O	S			
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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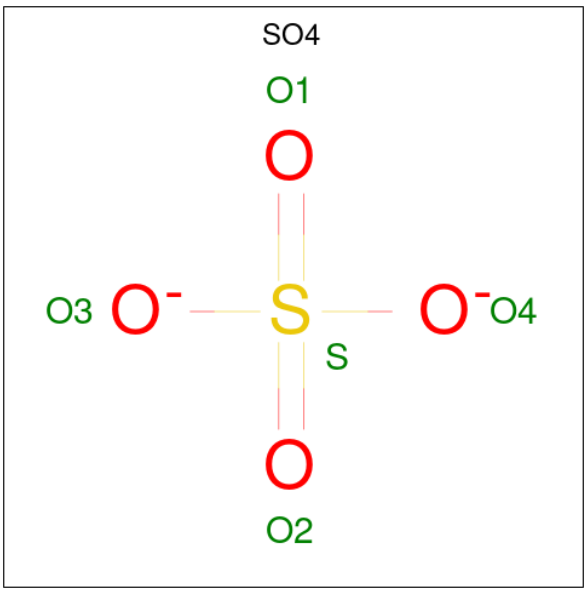
Chain	Residue	Modelled	Actual	Comment	Reference
F	317	HIS	-	expression tag	UNP C7HJU1
F	318	HIS	-	expression tag	UNP C7HJU1
F	319	HIS	-	expression tag	UNP C7HJU1
F	320	HIS	-	expression tag	UNP C7HJU1
F	321	HIS	-	expression tag	UNP C7HJU1
I	1	MET	-	initiating methionine	UNP C7HJU1
I	314	LEU	-	expression 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
			Total	Ca		
4	A	2	2	2	0	0
4	C	2	2	2	0	0
4	D	2	2	2	0	0
4	F	2	2	2	0	0
4	G	2	2	2	0	0
4	I	2	2	2	0	0
4	J	2	2	2	0	0
4	L	2	2	2	0	0

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



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

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

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

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

- Molecule 6 is water.

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

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: 61% 13% • 23%

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE GLU GLY ARG H21 M22 V25 L38 T49 L50 S53 D64 G65 R66 V67 D71 I80 L86 P87 I88

• Molecule 1: Glycoside hydrolase family 9

Chain D: 2% 49% 23% • 26%

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE GLU GLY ARG HIS M22 G23 D24 V25 G29 S33 T34 D35 L38 Y42 V43 L44 S48 T49 L50 S53 N58 A59 D60 R63 D64 G65 R66 V67 D71 R77 I80

K85 L86 PRO ILE

• Molecule 1: Glycoside hydrolase family 9

Chain G: 45% 25% 5% • 24%

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE GLU GLY ARG H21 M22 V25 S33 L38 L39 K40 R41 Y42 V47 S48 T49 L50 P51 D60 V61 D64 G65 R66 V67 N68 S69 S70 D71 V72 T73 R77 I80 L86 P87 ILE

• Molecule 1: Glycoside hydrolase family 9

Chain J: 3% 39% 31% 6% 25%

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE GLU GLY ARG H21 M22 G23 D24 V25 D28 G29 S33 T34 D35 L36 R41 Y42 L50 S53 K54 K57 N58 A59 D60 V61 G65 R66 V67 N68 S69 S70 D71 V72 L75 S76 R77

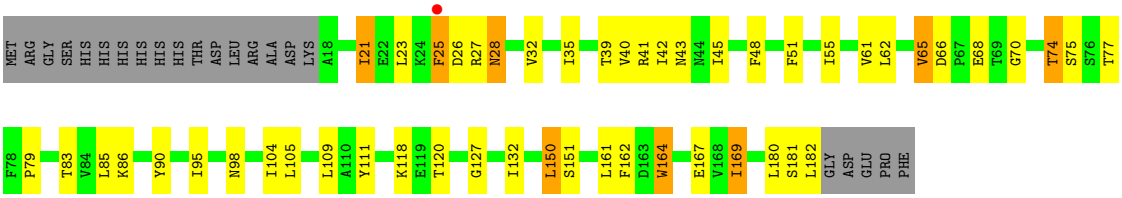
I80 R81 V82 I83 E84 K85 L86 PRO ILE

• Molecule 2: Scaffolding dockerin binding protein A

Chain B: % 77% 11% • 12%

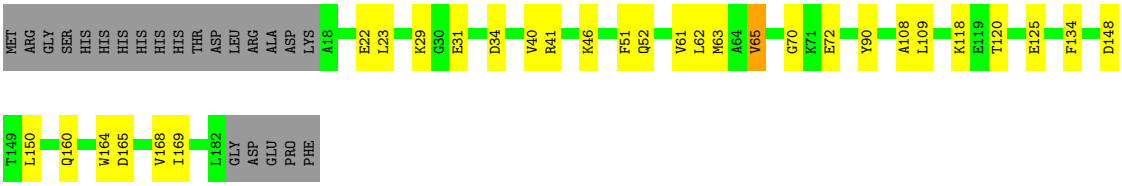
• Molecule 2: Scaffolding dockerin binding protein A

Chain E:



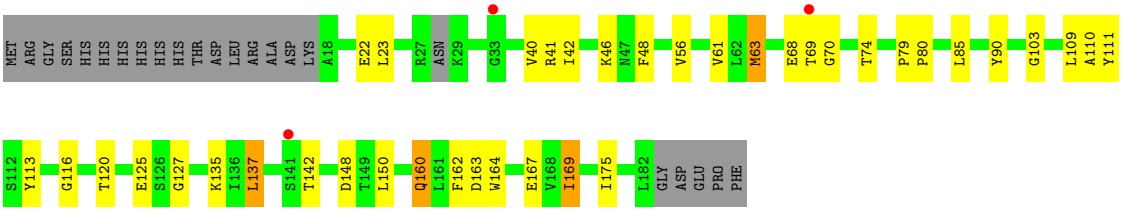
• Molecule 2: Scaffolding dockerin binding protein A

Chain H:



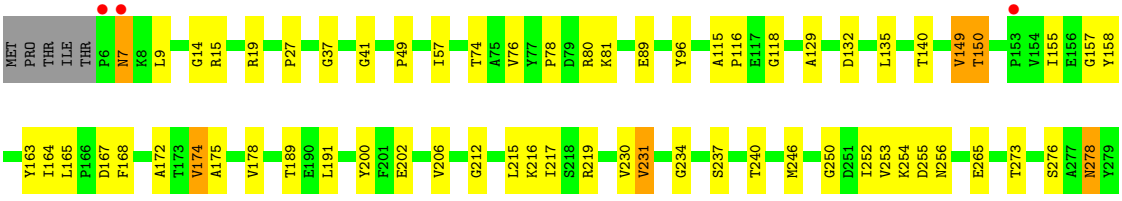
• Molecule 2: Scaffolding dockerin binding protein A

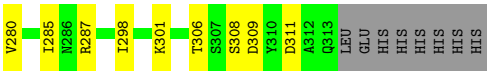
Chain K:



• Molecule 3: Cellulosome anchoring protein cohesin region

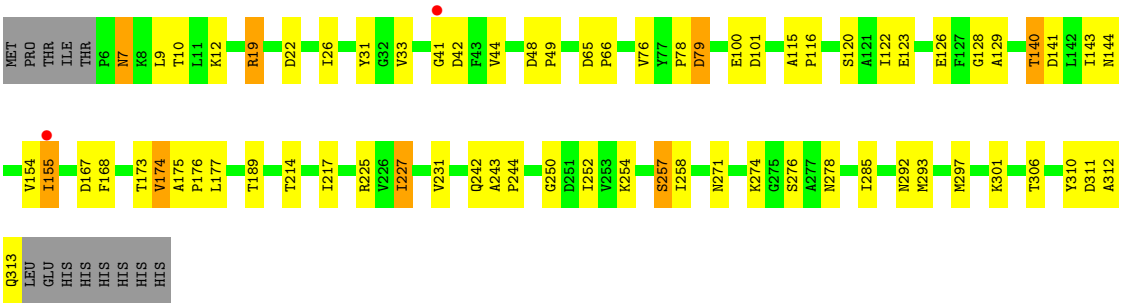
Chain C:





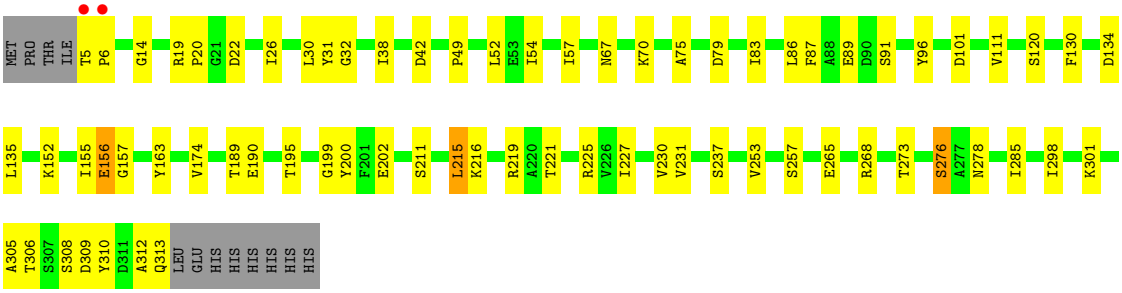
• Molecule 3: Cellulosome anchoring protein cohesin region

Chain F:



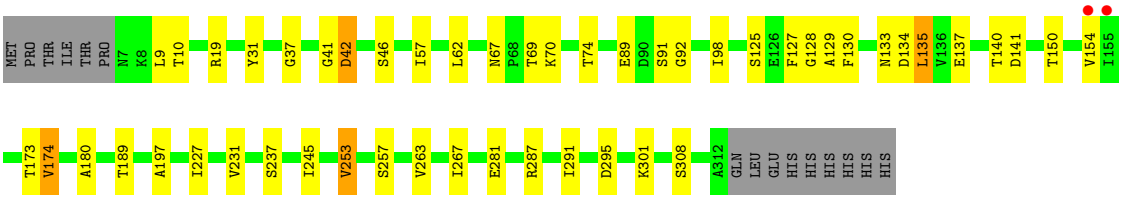
• Molecule 3: Cellulosome anchoring protein cohesin region

Chain I:



• Molecule 3: Cellulosome anchoring protein cohesin region

Chain L:



4 Data and refinement statistics (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) 99.5 (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]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	497	0	480	10	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (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
2:E:25[A]:PHE:N	2:E:25[A]:PHE:HD2	1.72	0.88
1:G:66:ARG:HG2	1:G:68:ASN:HD22	1.38	0.87
1:D:49:THR:OG1	1:D:50:LEU:N	2.07	0.87
3:F:276:SER:OG	5:F:413:SO4:O2	1.93	0.86
1:J:77:ARG:HB2	1:J:83:ILE:HD12	1.63	0.80
3:I:155:ILE:HD13	3:I:157:GLY:O	1.82	0.79
2:E:95:ILE:HD13	3:F:293:MET:HE1	1.66	0.78
3:I:155:ILE:HD12	3:I:156:GLU:N	2.03	0.74
3:I:67:ASN:HB2	3:I:70:LYS:HE2	1.69	0.74
3:L:134:ASP:O	3:L:135:LEU:HB2	1.88	0.74
1:G:86:LEU:HG	1:G:86:LEU:O	1.87	0.73
1:G:66:ARG:HG2	1:G:68:ASN:ND2	2.05	0.72
3:C:118:GLY:O	3:C:149:VAL:HG23	1.89	0.72
3:L:308:SER:N	5:L:407:SO4:O1	2.23	0.71
3:I:225:ARG:HG3	3:I:310:TYR:CD2	2.26	0.70
1:G:61:VAL:O	1:G:87:PRO:HD2	1.91	0.70
3:C:89:GLU:HG2	3:C:96:TYR:HB2	1.74	0.69
3:F:250:GLY:HA3	3:F:258:ILE:HD13	1.74	0.69
3:F:10:THR:HG22	3:F:141:ASP:HB2	1.74	0.68
2:E:74:THR:HG23	2:E:77:THR:OG1	1.94	0.68
3:F:9:LEU:HD23	3:F:140:THR:CG2	2.24	0.68
3:L:89:GLU:OE2	3:L:91:SER:OG	2.05	0.67
3:L:10:THR:HG22	3:L:141:ASP:HB2	1.77	0.67
1:A:25:VAL:HG12	1:A:38:LEU:HD23	1.78	0.66
1:J:33:SER:HB3	3:L:42:ASP:HB3	1.78	0.66
2:E:23:LEU:HD13	2:E:40:VAL:HG22	1.78	0.65
2:K:63:MET:HE2	2:K:135:LYS:HE2	1.78	0.65
2:E:90:TYR:OH	2:E:120:THR:HG21	1.96	0.65
3:I:89:GLU:HG2	3:I:96:TYR:HB2	1.79	0.65
2:E:26:ASP:OD1	2:E:27:ARG:N	2.31	0.64
1:G:60:ASP:OD2	1:G:64:ASP:N	2.31	0.63
1:D:23:GLY:H	1:D:58:ASN:HB3	1.62	0.63
3:I:273:THR:O	3:I:276:SER:HB3	1.98	0.63
2:H:41:ARG:NH2	5:H:202:SO4:O4	2.32	0.62
3:C:15:ARG:NH2	5:C:405:SO4:O2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:ASP:OD2	1:J:65:GLY:N	2.32	0.62
3:C:285:ILE:HG21	3:C:298:ILE:HG21	1.82	0.62
3:L:67:ASN:HB2	3:L:70:LYS:HD2	1.82	0.62
3:I:163:TYR:CE2	3:I:200:TYR:HB2	2.35	0.61
2:B:47:ASN:O	2:B:163:ASP:HA	2.00	0.61
2:K:163:ASP:HB3	2:K:169:ILE:HD11	1.83	0.61
2:K:167:GLU:OE2	3:L:301:LYS:NZ	2.34	0.60
1:G:66:ARG:CG	1:G:68:ASN:HD22	2.10	0.60
2:H:118:LYS:NZ	2:H:165:ASP:OD2	2.28	0.60
3:L:9:LEU:HB3	3:L:140:THR:HG22	1.83	0.60
1:A:49:THR:HG23	1:A:50:LEU:O	2.03	0.59
3:C:278:ASN:ND2	3:C:278:ASN:H	1.99	0.59
3:F:278:ASN:HB2	5:F:413:SO4:O4	2.03	0.59
3:C:163:TYR:CE2	3:C:200:TYR:HB2	2.38	0.58
3:F:167:ASP:O	3:F:168:PHE:HB3	2.04	0.58
3:C:7:ASN:O	3:C:7:ASN:ND2	2.25	0.58
1:G:41:ARG:HB3	1:G:47:VAL:HG13	1.85	0.58
2:B:23:LEU:HB3	2:B:177:PRO:HD3	1.86	0.57
2:B:146:PHE:HB2	2:B:176:GLN:HE22	1.68	0.57
2:E:95:ILE:HD13	3:F:293:MET:CE	2.34	0.57
3:C:155:ILE:HD12	3:C:157:GLY:O	2.05	0.57
3:C:41:GLY:HA2	3:C:129:ALA:O	2.05	0.57
1:G:22:MET:HB2	1:G:86:LEU:HD22	1.86	0.57
2:H:51:PHE:CE1	2:H:109:LEU:HB3	2.40	0.57
2:B:116:GLY:O	2:B:120:THR:HG23	2.04	0.57
3:F:10:THR:CG2	3:F:141:ASP:HB2	2.34	0.57
3:C:202:GLU:HG3	3:C:202:GLU:O	2.05	0.56
3:C:158:TYR:CE1	3:C:234:GLY:HA2	2.40	0.56
3:F:9:LEU:HB3	3:F:140:THR:HG22	1.88	0.56
2:E:61:VAL:HG12	2:E:62:LEU:HG	1.88	0.56
2:H:61:VAL:O	2:H:62:LEU:HD23	2.05	0.56
1:A:22:MET:HG3	1:A:87:PRO:HG3	1.88	0.56
2:H:52:GLN:HG3	2:H:108:ALA:HB2	1.88	0.56
1:J:67:VAL:HA	1:J:71:ASP:OD2	2.06	0.55
2:B:118:LYS:HA	2:B:164:TRP:CE3	2.41	0.55
3:F:123:GLU:HG2	3:F:144:ASN:HD22	1.72	0.55
3:F:79:ASP:OD1	3:F:79:ASP:N	2.26	0.55
1:J:21:HIS:CG	1:J:22:MET:N	2.73	0.55
1:J:42:TYR:CD1	1:J:50:LEU:HG	2.41	0.55
2:B:146:PHE:HB2	2:B:176:GLN:NE2	2.22	0.55
3:L:9:LEU:HD23	3:L:140:THR:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:TYR:CD1	1:G:50:LEU:HD13	2.42	0.54
2:E:151:SER:O	3:F:292:ASN:ND2	2.37	0.54
1:A:67:VAL:HA	1:A:71:ASP:OD2	2.07	0.54
3:L:263:VAL:O	3:L:267:ILE:HG12	2.08	0.54
1:A:38:LEU:HB2	3:C:135:LEU:HD23	1.89	0.53
1:J:25:VAL:HG23	1:J:35:ASP:HB3	1.90	0.53
3:C:298:ILE:O	3:C:301:LYS:HB2	2.08	0.53
1:G:86:LEU:O	1:G:86:LEU:CG	2.56	0.53
1:D:25:VAL:HG12	1:D:38:LEU:HD23	1.90	0.53
2:H:23:LEU:HD13	2:H:40:VAL:HG22	1.90	0.52
3:C:252:ILE:N	3:C:252:ILE:HD12	2.25	0.52
3:I:89:GLU:OE2	3:I:91:SER:OG	2.13	0.52
2:K:61:VAL:O	2:K:137:LEU:HB2	2.08	0.52
3:I:219:ARG:NE	5:I:405:SO4:O2	2.36	0.52
3:F:33:VAL:HG21	3:F:100:GLU:O	2.10	0.52
3:L:127:PHE:CE2	3:L:129:ALA:HA	2.45	0.52
3:L:174:VAL:HG21	3:L:287:ARG:HB2	1.92	0.52
2:E:41:ARG:NH1	5:E:202:SO4:O1	2.42	0.52
1:D:85:LYS:O	1:D:86:LEU:HB2	2.10	0.51
3:I:20:PRO:HA	3:I:111:VAL:HG12	1.92	0.51
3:I:134:ASP:O	3:I:135:LEU:HB2	2.10	0.51
3:C:287:ARG:HG2	3:C:287:ARG:HH11	1.75	0.51
1:G:67:VAL:HA	1:G:71:ASP:OD2	2.10	0.51
3:F:250:GLY:O	3:F:252:ILE:HG13	2.10	0.51
1:J:42:TYR:CE1	1:J:50:LEU:HG	2.45	0.51
3:I:26:ILE:HD12	3:I:26:ILE:N	2.25	0.51
2:E:167:GLU:OE2	3:F:301:LYS:NZ	2.29	0.51
3:F:225:ARG:HB2	3:F:310:TYR:CE2	2.46	0.51
3:I:225:ARG:HG3	3:I:310:TYR:CG	2.45	0.51
3:I:253:VAL:O	3:I:253:VAL:CG2	2.59	0.51
2:H:63:MET:HE3	2:H:72:GLU:HB2	1.93	0.51
3:I:86:LEU:HD12	3:I:87:PHE:N	2.26	0.51
1:J:22:MET:HE3	1:J:61:VAL:HA	1.93	0.50
1:J:57:LYS:O	1:J:59:ALA:N	2.42	0.50
3:I:298:ILE:HA	3:I:301:LYS:HD2	1.92	0.50
3:F:9:LEU:O	3:F:140:THR:HA	2.11	0.50
1:G:33:SER:HB3	3:I:42:ASP:HB3	1.94	0.50
1:D:24:ASP:HB3	1:D:58:ASN:HD22	1.77	0.50
1:G:38:LEU:HB2	3:I:135:LEU:HD23	1.94	0.50
2:E:83:THR:HA	2:E:86:LYS:HE3	1.94	0.50
1:G:80:ILE:HG13	3:I:75:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:90:TYR:OH	2:K:120:THR:HG21	2.11	0.50
3:L:41:GLY:HA2	3:L:129:ALA:O	2.12	0.49
2:B:119:GLU:HG3	2:B:119:GLU:O	2.12	0.49
3:L:57:ILE:HG21	3:L:74:THR:HG21	1.94	0.49
3:F:155:ILE:HG12	3:F:155:ILE:O	2.12	0.49
3:C:76:VAL:HG12	3:C:78:PRO:HD3	1.94	0.49
3:C:158:TYR:CD1	3:C:234:GLY:HA2	2.47	0.49
3:F:19:ARG:O	3:F:22:ASP:HB2	2.12	0.49
2:E:75:SER:HA	2:E:98:ASN:HB2	1.94	0.49
2:B:165:ASP:O	3:C:301:LYS:HE3	2.13	0.49
3:C:250:GLY:HA2	3:C:252:ILE:CD1	2.43	0.49
1:J:22:MET:CE	1:J:61:VAL:HA	2.43	0.49
2:B:23:LEU:HD13	2:B:40:VAL:HG22	1.94	0.48
1:J:80:ILE:HG22	1:J:82:VAL:H	1.79	0.48
2:E:65:VAL:HG13	2:E:70:GLY:HA2	1.94	0.48
1:J:21:HIS:CG	1:J:22:MET:H	2.31	0.48
1:J:80:ILE:HD12	1:J:80:ILE:HA	1.69	0.48
1:A:22:MET:CG	1:A:87:PRO:HG3	2.43	0.48
1:G:69:SER:O	1:G:72:VAL:HB	2.13	0.48
2:H:31:GLU:O	2:H:34:ASP:HB2	2.13	0.48
1:J:69:SER:O	1:J:72:VAL:HB	2.13	0.48
2:E:65:VAL:HG22	2:E:70:GLY:O	2.13	0.48
1:J:24:ASP:OD2	1:J:28:ASP:N	2.46	0.48
1:A:87:PRO:O	1:A:88:ILE:C	2.51	0.48
1:D:60:ASP:OD2	1:D:65:GLY:N	2.46	0.48
1:D:24:ASP:HA	1:D:35:ASP:OD2	2.14	0.48
3:F:26:ILE:HD13	3:F:122:ILE:CD1	2.43	0.48
3:F:115:ALA:HA	3:F:116:PRO:HD3	1.72	0.48
3:L:10:THR:OG1	3:L:31:TYR:HB2	2.13	0.48
2:E:151:SER:HB3	3:F:271:ASN:OD1	2.14	0.47
3:I:31:TYR:HA	3:I:101:ASP:OD2	2.13	0.47
2:E:25[A]:PHE:HD1	2:E:180:LEU:HD11	1.79	0.47
3:C:273:THR:O	3:C:276:SER:N	2.45	0.47
3:I:312:ALA:O	3:I:313:GLN:HB2	2.14	0.47
1:G:25:VAL:HG12	1:G:38:LEU:HD23	1.95	0.47
1:A:86:LEU:O	1:A:87:PRO:C	2.53	0.47
2:B:154:GLY:HA2	3:L:173:THR:OG1	2.15	0.47
3:C:306:THR:O	3:C:309:ASP:HB2	2.15	0.47
2:E:45:ILE:HG22	2:E:169:ILE:HD12	1.97	0.47
2:K:68:GLU:O	2:K:70:GLY:N	2.48	0.47
3:I:215:LEU:HD22	3:I:230:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:22:GLU:HG3	2:K:175:ILE:HB	1.97	0.46
1:J:41:ARG:NH2	3:L:133:ASN:O	2.48	0.46
1:D:77:ARG:O	1:D:80:ILE:HG22	2.15	0.46
3:F:9:LEU:HD23	3:F:140:THR:HG21	1.97	0.46
3:I:49:PRO:HA	3:I:52:LEU:O	2.14	0.46
2:K:48:PHE:CE1	2:K:85:LEU:HD11	2.51	0.46
3:C:273:THR:O	3:C:276:SER:HB3	2.16	0.46
2:E:21:ILE:HG13	2:E:42:ILE:HG22	1.97	0.46
3:F:65:ASP:OD1	3:F:66:PRO:HD2	2.16	0.46
3:I:38:ILE:HG21	3:I:130:PHE:HD2	1.80	0.46
2:K:113:TYR:CE2	2:K:116:GLY:HA3	2.51	0.46
1:D:33:SER:HB3	3:F:42:ASP:HB3	1.98	0.46
3:I:57:ILE:N	3:I:57:ILE:HD12	2.30	0.46
3:C:254:LYS:HE3	3:C:254:LYS:HB3	1.70	0.46
3:C:278:ASN:ND2	3:C:278:ASN:N	2.64	0.46
2:E:85:LEU:HA	2:E:111:TYR:CZ	2.51	0.46
3:F:173:THR:O	3:F:173:THR:HG22	2.16	0.46
3:I:257:SER:HA	3:I:305:ALA:O	2.16	0.46
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.65	0.45
3:C:14:GLY:HA3	3:C:27:PRO:HD2	1.99	0.45
3:F:254:LYS:HB3	3:F:254:LYS:HE2	1.60	0.45
1:G:50:LEU:HA	1:G:51:PRO:HD3	1.77	0.45
2:K:160:GLN:HG2	2:K:162:PHE:CZ	2.52	0.45
3:C:215:LEU:HD13	3:C:230:VAL:HG21	1.98	0.45
1:G:22:MET:HG2	1:G:86:LEU:HD13	1.97	0.45
2:E:85:LEU:HA	2:E:111:TYR:OH	2.17	0.45
1:J:85:LYS:O	1:J:86:LEU:HB3	2.16	0.45
2:K:41:ARG:HB2	2:K:127:GLY:O	2.17	0.45
3:F:257:SER:OG	3:F:306:THR:HG22	2.17	0.45
3:I:19:ARG:HG3	3:I:22:ASP:OD2	2.16	0.45
3:F:42:ASP:OD1	3:F:128:GLY:HA3	2.17	0.45
2:K:63:MET:HE2	2:K:63:MET:HB3	1.96	0.44
1:D:67:VAL:HA	1:D:71:ASP:OD2	2.17	0.44
3:I:253:VAL:O	3:I:253:VAL:HG22	2.18	0.44
3:L:127:PHE:CZ	3:L:130:PHE:HD1	2.36	0.44
3:C:37:GLY:O	3:C:132:ASP:HA	2.17	0.44
2:E:74:THR:OG1	2:E:75:SER:N	2.50	0.44
3:I:32:GLY:N	3:I:101:ASP:OD2	2.41	0.44
2:K:109:LEU:HG	2:K:110:ALA:N	2.32	0.44
2:E:66:ASP:OD1	2:E:68:GLU:N	2.44	0.44
2:K:85:LEU:HD12	2:K:109:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ALA:O	3:C:174:VAL:N	2.51	0.44
3:L:46:SER:HB3	3:L:125:SER:HB2	1.99	0.44
3:F:123:GLU:HB3	3:F:144:ASN:ND2	2.33	0.44
1:G:73:THR:O	1:G:77:ARG:HG3	2.18	0.44
1:G:86:LEU:C	1:G:86:LEU:HD12	2.38	0.44
3:F:41:GLY:HA2	3:F:129:ALA:O	2.18	0.44
3:F:175:ALA:HB3	3:F:176:PRO:HD3	2.00	0.44
3:I:86:LEU:HD12	3:I:87:PHE:H	1.83	0.44
3:I:202:GLU:O	3:I:202:GLU:HG3	2.16	0.44
1:J:36:LEU:HA	1:J:75:LEU:HD23	2.00	0.44
3:C:57:ILE:HG21	3:C:74:THR:HG21	1.99	0.43
2:E:79:PRO:HB3	2:E:132:ILE:HG12	2.00	0.43
2:K:23:LEU:HD13	2:K:40:VAL:HG22	1.99	0.43
3:C:212:GLY:HA2	3:C:231:VAL:HA	2.00	0.43
2:H:90:TYR:OH	2:H:120:THR:HG21	2.17	0.43
3:L:227:ILE:CD1	3:L:245:ILE:HD13	2.49	0.43
3:C:9:LEU:HD23	3:C:140:THR:OG1	2.18	0.43
3:F:12:LYS:HD2	3:F:143:ILE:HG21	2.00	0.43
3:F:44:VAL:HB	3:F:126:GLU:HB2	2.01	0.43
3:F:312:ALA:O	3:F:313:GLN:HB2	2.18	0.43
2:B:51:PHE:CE1	2:B:109:LEU:HB3	2.53	0.43
3:C:175:ALA:HA	3:C:178:VAL:CG2	2.49	0.43
2:E:55:ILE:HB	2:E:105:LEU:HB2	2.00	0.43
3:F:31:TYR:HA	3:F:101:ASP:CG	2.38	0.43
3:C:115:ALA:HA	3:C:116:PRO:HD3	1.90	0.43
2:E:35:ILE:O	2:E:35:ILE:HG22	2.18	0.43
3:F:48:ASP:HA	3:F:49:PRO:HD2	1.90	0.43
2:H:46:LYS:HA	2:H:125:GLU:OE1	2.19	0.43
2:H:65:VAL:CG1	2:H:70:GLY:HA2	2.48	0.43
3:F:167:ASP:OD2	3:F:167:ASP:C	2.57	0.43
2:E:51:PHE:HB2	2:E:161:LEU:HD23	2.01	0.43
3:I:26:ILE:HD12	3:I:26:ILE:H	1.84	0.43
3:I:30:LEU:HD23	3:I:30:LEU:HA	1.78	0.43
2:K:79:PRO:HA	2:K:80:PRO:HD3	1.91	0.43
3:I:54:ILE:HD12	3:I:83:ILE:HD11	2.01	0.43
3:F:26:ILE:HD13	3:F:122:ILE:HD12	2.00	0.42
2:E:66:ASP:OD1	2:E:66:ASP:C	2.57	0.42
3:I:306:THR:O	3:I:309:ASP:HB2	2.20	0.42
3:L:130:PHE:O	3:L:137:GLU:HA	2.19	0.42
2:K:42:ILE:O	2:K:42:ILE:HG13	2.18	0.42
3:L:291:ILE:HA	3:L:295:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:ASP:O	3:C:168:PHE:HB3	2.20	0.42
3:C:89:GLU:HG3	3:C:96:TYR:C	2.40	0.42
1:D:42:TYR:CZ	1:D:50:LEU:HD22	2.54	0.42
2:K:68:GLU:C	2:K:70:GLY:H	2.23	0.42
3:C:191:LEU:HD13	3:C:206:VAL:HG22	2.02	0.42
2:E:48:PHE:CE1	2:E:85:LEU:HD11	2.54	0.42
1:J:54:LYS:O	1:J:57:LYS:N	2.48	0.42
3:C:164:ILE:HD13	3:C:217:ILE:HG21	2.01	0.42
2:E:27:ARG:HH11	2:E:28:ASN:H	1.67	0.42
2:H:65:VAL:HG13	2:H:70:GLY:HA2	2.01	0.42
3:L:37:GLY:O	3:L:133:ASN:N	2.52	0.42
3:F:243:ALA:N	3:F:244:PRO:HD3	2.35	0.42
3:C:19:ARG:HA	3:C:150:THR:O	2.20	0.41
2:E:162:PHE:CG	3:F:297:MET:HG3	2.55	0.41
1:J:21:HIS:CD2	1:J:22:MET:H	2.38	0.41
1:J:70:SER:C	1:J:72:VAL:N	2.72	0.41
3:L:9:LEU:O	3:L:140:THR:HA	2.20	0.41
2:E:118:LYS:HA	2:E:164:TRP:CE3	2.54	0.41
1:J:66:ARG:HG2	1:J:68:ASN:HD22	1.85	0.41
3:I:273:THR:H	3:I:276:SER:HB3	1.85	0.41
3:C:219:ARG:NE	5:C:404:SO4:O3	2.34	0.41
3:F:274:LYS:HE3	3:F:274:LYS:HB2	1.96	0.41
2:K:56:VAL:HA	2:K:103:GLY:O	2.20	0.41
3:L:127:PHE:HZ	3:L:130:PHE:HD1	1.68	0.41
1:D:58:ASN:OD1	1:D:58:ASN:N	2.54	0.41
2:H:62:LEU:HD13	2:H:134:PHE:HB3	2.02	0.41
3:I:195:THR:HB	3:I:199:GLY:HA2	2.03	0.41
3:L:135:LEU:N	3:L:135:LEU:CD1	2.84	0.41
3:I:265:GLU:OE2	3:I:268:ARG:NH1	2.54	0.41
3:C:49:PRO:CD	3:C:81:LYS:HG2	2.51	0.41
3:C:255:ASP:O	3:C:256:ASN:HB2	2.19	0.41
2:E:41:ARG:HB2	2:E:127:GLY:O	2.20	0.41
1:J:70:SER:O	1:J:71:ASP:C	2.58	0.41
2:E:27:ARG:HA	2:E:27:ARG:HD2	1.67	0.41
3:F:26:ILE:CD1	3:F:122:ILE:CD1	2.99	0.41
2:H:22:GLU:HG2	2:H:23:LEU:N	2.35	0.41
1:J:41:ARG:HG3	3:L:92:GLY:O	2.21	0.41
3:L:180:ALA:HB2	3:L:197:ALA:HA	2.02	0.41
3:L:253:VAL:O	3:L:253:VAL:CG2	2.68	0.41
2:B:113:TYR:CE2	2:B:116:GLY:HA3	2.56	0.41
3:C:273:THR:H	3:C:276:SER:CB	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:76:VAL:HG12	3:F:78:PRO:HD3	2.03	0.41
3:C:165:LEU:O	3:C:246:MET:HA	2.21	0.40
1:G:39:LEU:HA	1:G:39:LEU:HD12	1.77	0.40
2:K:85:LEU:HA	2:K:111:TYR:CZ	2.56	0.40
3:F:174:VAL:HG22	3:F:177:LEU:HD12	2.04	0.40
3:I:5:THR:N	3:I:6:PRO:HD3	2.36	0.40
3:L:128:GLY:O	3:L:129:ALA:HB2	2.20	0.40
3:F:217:ILE:HD11	3:F:227:ILE:HD11	2.04	0.40
2:B:51:PHE:HE1	2:B:109:LEU:HD23	1.87	0.40
1:D:48:SER:HA	1:D:49:THR:HA	1.40	0.40
2:E:150:LEU:HA	2:E:150:LEU:HD12	1.83	0.40
2:K:46:LYS:HA	2:K:125:GLU:OE1	2.21	0.40
3:L:62:LEU:HD13	3:L:98:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
3	I	156	GLU
3	I	276	SER
2	K	69	THR
1	G	50	LEU
1	A	86	LEU
1	J	71	ASP
2	B	32	VAL
3	F	285	ILE
3	I	14	GLY
3	C	280	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%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	53	SER
1	A	64	ASP
1	A	66	ARG
1	A	80	ILE
2	B	65	VAL
2	B	112	SER
2	B	137	LEU
2	B	164	TRP
3	C	7	ASN
3	C	80	ARG
3	C	149	VAL
3	C	150	THR
3	C	174	VAL
3	C	189	THR
3	C	216	LYS
3	C	231	VAL
3	C	237	SER
3	C	240	THR
3	C	253	VAL
3	C	265	GLU
3	C	278	ASN
3	C	308	SER
3	C	311	ASP
1	D	44	LEU
1	D	50	LEU
1	D	53	SER
1	D	58	ASN
1	D	63	ARG

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Mol	Chain	Res	Type
2	E	21	ILE
2	E	25[A]	PHE
2	E	25[B]	PHE
2	E	28	ASN
2	E	39	THR
2	E	43	ASN
2	E	65	VAL
2	E	74	THR
2	E	104	ILE
2	E	109	LEU
2	E	150	LEU
2	E	164	TRP
2	E	169	ILE
2	E	181	SER
2	E	182	LEU
3	F	7	ASN
3	F	19	ARG
3	F	79	ASP
3	F	120	SER
3	F	140	THR
3	F	154	VAL
3	F	155	ILE
3	F	174	VAL
3	F	189	THR
3	F	214	THR
3	F	227	ILE
3	F	231	VAL
3	F	242	GLN
3	F	257	SER
3	F	311	ASP
1	G	21	HIS
1	G	22	MET
1	G	47	VAL
1	G	48	SER
1	G	49	THR
1	G	50	LEU
1	G	86	LEU
2	H	29	LYS
2	H	65	VAL
2	H	148	ASP
2	H	150	LEU
2	H	160	GLN

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Mol	Chain	Res	Type
2	H	164	TRP
2	H	168	VAL
2	H	169	ILE
3	I	79	ASP
3	I	120	SER
3	I	174	VAL
3	I	189	THR
3	I	190	GLU
3	I	211	SER
3	I	215	LEU
3	I	216	LYS
3	I	221	THR
3	I	227	ILE
3	I	231	VAL
3	I	237	SER
3	I	278	ASN
3	I	285	ILE
3	I	308	SER
1	J	66	ARG
1	J	77	ARG
1	J	80	ILE
1	J	86	LEU
2	K	63	MET
2	K	74	THR
2	K	137	LEU
2	K	142	THR
2	K	148	ASP
2	K	150	LEU
2	K	160	GLN
2	K	164	TRP
2	K	169	ILE
3	L	19	ARG
3	L	42	ASP
3	L	69	THR
3	L	135	LEU
3	L	150	THR
3	L	154	VAL
3	L	174	VAL
3	L	189	THR
3	L	231	VAL
3	L	237	SER
3	L	253	VAL

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Mol	Chain	Res	Type
3	L	257	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	278	ASN
2	E	28	ASN
3	F	144	ASN
3	I	313	GLN
1	J	21	HIS
1	J	68	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 monosaccharides 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	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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
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 (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%)	-0.25	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%)

All (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
1	J	29	GLY	2.5
2	K	33	GLY	2.4
1	J	53	SER	2.3
2	B	18	ALA	2.3
3	C	6	PRO	2.3
3	L	154	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	25[A]	PHE	2.2
3	F	155	ILE	2.2
3	L	155	ILE	2.2
2	K	141	SER	2.1
3	F	41	GLY	2.1
3	C	7	ASN	2.1
1	D	65	GLY	2.0
3	I	6	PRO	2.0

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 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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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.