



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:21 PM BST

PDB ID : 6NER  
Title : Synthetic Haliangium ochraceum BMC shell  
Authors : Sutter, M.; McGuire, S.; Aussignargues, C.; Kerfeld, C.A.  
Deposited on : 2018-12-18  
Resolution : 3.59 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

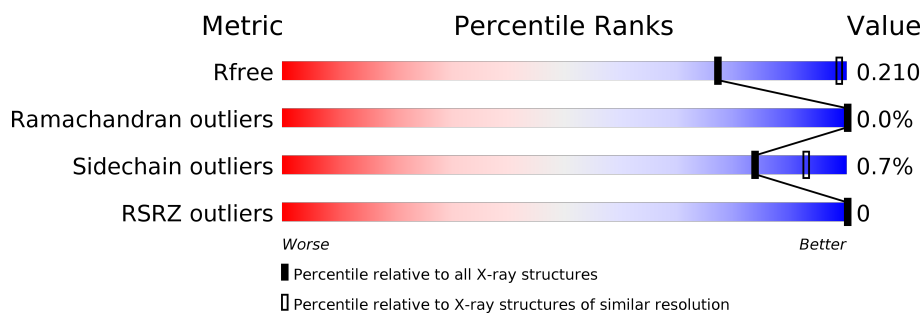
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 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.

















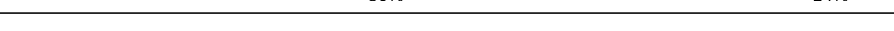








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	<div> <div>86%</div> <div>13%</div> </div>
1	B	213	<div> <div>86%</div> <div>13%</div> </div>
1	C	213	<div> <div>86%</div> <div>13%</div> </div>
1	D	213	<div> <div>85%</div> <div>15%</div> </div>
1	E	213	<div> <div>87%</div> <div>13%</div> </div>
1	F	213	<div> <div>86%</div> <div>14%</div> </div>
1	G	213	<div> <div>85%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	213	 87% 13%
1	I	213	 86% 14%
1	J	213	 86% 14%
1	K	213	 87% 13%
1	L	213	 86% 14%
1	M	213	 85% 14%
1	N	213	 86% 14%
1	O	213	 86% 14%
1	P	213	 85% 14%
1	Q	213	 86% 14%
1	R	213	 86% 14%
1	S	213	 85% 15%
1	T	213	 86% 14%
1	U	213	 86% 14%
1	V	213	 86% 13%
1	W	213	 86% 14%
1	X	213	 86% 14%
1	Y	213	 86% 13%
1	Z	213	 86% 13%
1	a	213	 86% 14%
1	b	213	 85% 15%
1	c	213	 86% 13%
1	d	213	 86% 13%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39510 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 BMC-H tandem fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	B	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	C	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	D	182	Total	C	N	O	S	0	0	0
			1304	818	238	242	6			
1	E	186	Total	C	N	O	S	0	0	0
			1324	830	242	246	6			
1	F	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	G	183	Total	C	N	O	S	0	0	0
			1309	821	239	243	6			
1	H	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	I	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	J	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	K	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	L	183	Total	C	N	O	S	0	0	0
			1311	823	239	243	6			
1	M	183	Total	C	N	O	S	0	0	0
			1311	823	239	243	6			
1	N	183	Total	C	N	O	S	0	0	0
			1311	823	239	243	6			
1	O	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	P	183	Total	C	N	O	S	0	0	0
			1309	821	239	243	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	R	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	S	182	Total	C	N	O	S	0	0	0
			1304	818	238	242	6			
1	T	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	U	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	V	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	W	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	X	184	Total	C	N	O	S	0	0	0
			1315	825	240	244	6			
1	Y	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	Z	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	a	184	Total	C	N	O	S	0	0	0
			1316	826	240	244	6			
1	b	182	Total	C	N	O	S	0	0	0
			1302	816	238	242	6			
1	c	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			
1	d	185	Total	C	N	O	S	0	0	0
			1320	828	241	245	6			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	LEU	-	linker	UNP D0LID5
A	101	ASP	-	linker	UNP D0LID5
A	102	ALA	-	linker	UNP D0LID5
A	103	PRO	-	linker	UNP D0LID5
A	104	VAL	-	linker	UNP D0LID5
A	105	VAL	-	linker	UNP D0LID5
A	106	ALA	-	linker	UNP D0LID5
A	107	ASP	-	linker	UNP D0LID5
A	108	ALA	-	linker	UNP D0LID5
A	109	TRP	-	linker	UNP D0LID5
A	110	GLU	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	111	GLU	-	linker	UNP D0LID5
A	112	ASP	-	linker	UNP D0LID5
A	113	THR	-	linker	UNP D0LID5
A	114	GLU	-	linker	UNP D0LID5
A	115	SER	-	linker	UNP D0LID5
B	100	LEU	-	linker	UNP D0LID5
B	101	ASP	-	linker	UNP D0LID5
B	102	ALA	-	linker	UNP D0LID5
B	103	PRO	-	linker	UNP D0LID5
B	104	VAL	-	linker	UNP D0LID5
B	105	VAL	-	linker	UNP D0LID5
B	106	ALA	-	linker	UNP D0LID5
B	107	ASP	-	linker	UNP D0LID5
B	108	ALA	-	linker	UNP D0LID5
B	109	TRP	-	linker	UNP D0LID5
B	110	GLU	-	linker	UNP D0LID5
B	111	GLU	-	linker	UNP D0LID5
B	112	ASP	-	linker	UNP D0LID5
B	113	THR	-	linker	UNP D0LID5
B	114	GLU	-	linker	UNP D0LID5
B	115	SER	-	linker	UNP D0LID5
C	100	LEU	-	linker	UNP D0LID5
C	101	ASP	-	linker	UNP D0LID5
C	102	ALA	-	linker	UNP D0LID5
C	103	PRO	-	linker	UNP D0LID5
C	104	VAL	-	linker	UNP D0LID5
C	105	VAL	-	linker	UNP D0LID5
C	106	ALA	-	linker	UNP D0LID5
C	107	ASP	-	linker	UNP D0LID5
C	108	ALA	-	linker	UNP D0LID5
C	109	TRP	-	linker	UNP D0LID5
C	110	GLU	-	linker	UNP D0LID5
C	111	GLU	-	linker	UNP D0LID5
C	112	ASP	-	linker	UNP D0LID5
C	113	THR	-	linker	UNP D0LID5
C	114	GLU	-	linker	UNP D0LID5
C	115	SER	-	linker	UNP D0LID5
D	100	LEU	-	linker	UNP D0LID5
D	101	ASP	-	linker	UNP D0LID5
D	102	ALA	-	linker	UNP D0LID5
D	103	PRO	-	linker	UNP D0LID5
D	104	VAL	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	105	VAL	-	linker	UNP D0LID5
D	106	ALA	-	linker	UNP D0LID5
D	107	ASP	-	linker	UNP D0LID5
D	108	ALA	-	linker	UNP D0LID5
D	109	TRP	-	linker	UNP D0LID5
D	110	GLU	-	linker	UNP D0LID5
D	111	GLU	-	linker	UNP D0LID5
D	112	ASP	-	linker	UNP D0LID5
D	113	THR	-	linker	UNP D0LID5
D	114	GLU	-	linker	UNP D0LID5
D	115	SER	-	linker	UNP D0LID5
E	100	LEU	-	linker	UNP D0LID5
E	101	ASP	-	linker	UNP D0LID5
E	102	ALA	-	linker	UNP D0LID5
E	103	PRO	-	linker	UNP D0LID5
E	104	VAL	-	linker	UNP D0LID5
E	105	VAL	-	linker	UNP D0LID5
E	106	ALA	-	linker	UNP D0LID5
E	107	ASP	-	linker	UNP D0LID5
E	108	ALA	-	linker	UNP D0LID5
E	109	TRP	-	linker	UNP D0LID5
E	110	GLU	-	linker	UNP D0LID5
E	111	GLU	-	linker	UNP D0LID5
E	112	ASP	-	linker	UNP D0LID5
E	113	THR	-	linker	UNP D0LID5
E	114	GLU	-	linker	UNP D0LID5
E	115	SER	-	linker	UNP D0LID5
F	100	LEU	-	linker	UNP D0LID5
F	101	ASP	-	linker	UNP D0LID5
F	102	ALA	-	linker	UNP D0LID5
F	103	PRO	-	linker	UNP D0LID5
F	104	VAL	-	linker	UNP D0LID5
F	105	VAL	-	linker	UNP D0LID5
F	106	ALA	-	linker	UNP D0LID5
F	107	ASP	-	linker	UNP D0LID5
F	108	ALA	-	linker	UNP D0LID5
F	109	TRP	-	linker	UNP D0LID5
F	110	GLU	-	linker	UNP D0LID5
F	111	GLU	-	linker	UNP D0LID5
F	112	ASP	-	linker	UNP D0LID5
F	113	THR	-	linker	UNP D0LID5
F	114	GLU	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	115	SER	-	linker	UNP D0LID5
G	100	LEU	-	linker	UNP D0LID5
G	101	ASP	-	linker	UNP D0LID5
G	102	ALA	-	linker	UNP D0LID5
G	103	PRO	-	linker	UNP D0LID5
G	104	VAL	-	linker	UNP D0LID5
G	105	VAL	-	linker	UNP D0LID5
G	106	ALA	-	linker	UNP D0LID5
G	107	ASP	-	linker	UNP D0LID5
G	108	ALA	-	linker	UNP D0LID5
G	109	TRP	-	linker	UNP D0LID5
G	110	GLU	-	linker	UNP D0LID5
G	111	GLU	-	linker	UNP D0LID5
G	112	ASP	-	linker	UNP D0LID5
G	113	THR	-	linker	UNP D0LID5
G	114	GLU	-	linker	UNP D0LID5
G	115	SER	-	linker	UNP D0LID5
H	100	LEU	-	linker	UNP D0LID5
H	101	ASP	-	linker	UNP D0LID5
H	102	ALA	-	linker	UNP D0LID5
H	103	PRO	-	linker	UNP D0LID5
H	104	VAL	-	linker	UNP D0LID5
H	105	VAL	-	linker	UNP D0LID5
H	106	ALA	-	linker	UNP D0LID5
H	107	ASP	-	linker	UNP D0LID5
H	108	ALA	-	linker	UNP D0LID5
H	109	TRP	-	linker	UNP D0LID5
H	110	GLU	-	linker	UNP D0LID5
H	111	GLU	-	linker	UNP D0LID5
H	112	ASP	-	linker	UNP D0LID5
H	113	THR	-	linker	UNP D0LID5
H	114	GLU	-	linker	UNP D0LID5
H	115	SER	-	linker	UNP D0LID5
I	100	LEU	-	linker	UNP D0LID5
I	101	ASP	-	linker	UNP D0LID5
I	102	ALA	-	linker	UNP D0LID5
I	103	PRO	-	linker	UNP D0LID5
I	104	VAL	-	linker	UNP D0LID5
I	105	VAL	-	linker	UNP D0LID5
I	106	ALA	-	linker	UNP D0LID5
I	107	ASP	-	linker	UNP D0LID5
I	108	ALA	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	109	TRP	-	linker	UNP D0LID5
I	110	GLU	-	linker	UNP D0LID5
I	111	GLU	-	linker	UNP D0LID5
I	112	ASP	-	linker	UNP D0LID5
I	113	THR	-	linker	UNP D0LID5
I	114	GLU	-	linker	UNP D0LID5
I	115	SER	-	linker	UNP D0LID5
J	100	LEU	-	linker	UNP D0LID5
J	101	ASP	-	linker	UNP D0LID5
J	102	ALA	-	linker	UNP D0LID5
J	103	PRO	-	linker	UNP D0LID5
J	104	VAL	-	linker	UNP D0LID5
J	105	VAL	-	linker	UNP D0LID5
J	106	ALA	-	linker	UNP D0LID5
J	107	ASP	-	linker	UNP D0LID5
J	108	ALA	-	linker	UNP D0LID5
J	109	TRP	-	linker	UNP D0LID5
J	110	GLU	-	linker	UNP D0LID5
J	111	GLU	-	linker	UNP D0LID5
J	112	ASP	-	linker	UNP D0LID5
J	113	THR	-	linker	UNP D0LID5
J	114	GLU	-	linker	UNP D0LID5
J	115	SER	-	linker	UNP D0LID5
K	100	LEU	-	linker	UNP D0LID5
K	101	ASP	-	linker	UNP D0LID5
K	102	ALA	-	linker	UNP D0LID5
K	103	PRO	-	linker	UNP D0LID5
K	104	VAL	-	linker	UNP D0LID5
K	105	VAL	-	linker	UNP D0LID5
K	106	ALA	-	linker	UNP D0LID5
K	107	ASP	-	linker	UNP D0LID5
K	108	ALA	-	linker	UNP D0LID5
K	109	TRP	-	linker	UNP D0LID5
K	110	GLU	-	linker	UNP D0LID5
K	111	GLU	-	linker	UNP D0LID5
K	112	ASP	-	linker	UNP D0LID5
K	113	THR	-	linker	UNP D0LID5
K	114	GLU	-	linker	UNP D0LID5
K	115	SER	-	linker	UNP D0LID5
L	100	LEU	-	linker	UNP D0LID5
L	101	ASP	-	linker	UNP D0LID5
L	102	ALA	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
L	103	PRO	-	linker	UNP D0LID5
L	104	VAL	-	linker	UNP D0LID5
L	105	VAL	-	linker	UNP D0LID5
L	106	ALA	-	linker	UNP D0LID5
L	107	ASP	-	linker	UNP D0LID5
L	108	ALA	-	linker	UNP D0LID5
L	109	TRP	-	linker	UNP D0LID5
L	110	GLU	-	linker	UNP D0LID5
L	111	GLU	-	linker	UNP D0LID5
L	112	ASP	-	linker	UNP D0LID5
L	113	THR	-	linker	UNP D0LID5
L	114	GLU	-	linker	UNP D0LID5
L	115	SER	-	linker	UNP D0LID5
M	100	LEU	-	linker	UNP D0LID5
M	101	ASP	-	linker	UNP D0LID5
M	102	ALA	-	linker	UNP D0LID5
M	103	PRO	-	linker	UNP D0LID5
M	104	VAL	-	linker	UNP D0LID5
M	105	VAL	-	linker	UNP D0LID5
M	106	ALA	-	linker	UNP D0LID5
M	107	ASP	-	linker	UNP D0LID5
M	108	ALA	-	linker	UNP D0LID5
M	109	TRP	-	linker	UNP D0LID5
M	110	GLU	-	linker	UNP D0LID5
M	111	GLU	-	linker	UNP D0LID5
M	112	ASP	-	linker	UNP D0LID5
M	113	THR	-	linker	UNP D0LID5
M	114	GLU	-	linker	UNP D0LID5
M	115	SER	-	linker	UNP D0LID5
N	100	LEU	-	linker	UNP D0LID5
N	101	ASP	-	linker	UNP D0LID5
N	102	ALA	-	linker	UNP D0LID5
N	103	PRO	-	linker	UNP D0LID5
N	104	VAL	-	linker	UNP D0LID5
N	105	VAL	-	linker	UNP D0LID5
N	106	ALA	-	linker	UNP D0LID5
N	107	ASP	-	linker	UNP D0LID5
N	108	ALA	-	linker	UNP D0LID5
N	109	TRP	-	linker	UNP D0LID5
N	110	GLU	-	linker	UNP D0LID5
N	111	GLU	-	linker	UNP D0LID5
N	112	ASP	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
N	113	THR	-	linker	UNP D0LID5
N	114	GLU	-	linker	UNP D0LID5
N	115	SER	-	linker	UNP D0LID5
O	100	LEU	-	linker	UNP D0LID5
O	101	ASP	-	linker	UNP D0LID5
O	102	ALA	-	linker	UNP D0LID5
O	103	PRO	-	linker	UNP D0LID5
O	104	VAL	-	linker	UNP D0LID5
O	105	VAL	-	linker	UNP D0LID5
O	106	ALA	-	linker	UNP D0LID5
O	107	ASP	-	linker	UNP D0LID5
O	108	ALA	-	linker	UNP D0LID5
O	109	TRP	-	linker	UNP D0LID5
O	110	GLU	-	linker	UNP D0LID5
O	111	GLU	-	linker	UNP D0LID5
O	112	ASP	-	linker	UNP D0LID5
O	113	THR	-	linker	UNP D0LID5
O	114	GLU	-	linker	UNP D0LID5
O	115	SER	-	linker	UNP D0LID5
P	100	LEU	-	linker	UNP D0LID5
P	101	ASP	-	linker	UNP D0LID5
P	102	ALA	-	linker	UNP D0LID5
P	103	PRO	-	linker	UNP D0LID5
P	104	VAL	-	linker	UNP D0LID5
P	105	VAL	-	linker	UNP D0LID5
P	106	ALA	-	linker	UNP D0LID5
P	107	ASP	-	linker	UNP D0LID5
P	108	ALA	-	linker	UNP D0LID5
P	109	TRP	-	linker	UNP D0LID5
P	110	GLU	-	linker	UNP D0LID5
P	111	GLU	-	linker	UNP D0LID5
P	112	ASP	-	linker	UNP D0LID5
P	113	THR	-	linker	UNP D0LID5
P	114	GLU	-	linker	UNP D0LID5
P	115	SER	-	linker	UNP D0LID5
Q	100	LEU	-	linker	UNP D0LID5
Q	101	ASP	-	linker	UNP D0LID5
Q	102	ALA	-	linker	UNP D0LID5
Q	103	PRO	-	linker	UNP D0LID5
Q	104	VAL	-	linker	UNP D0LID5
Q	105	VAL	-	linker	UNP D0LID5
Q	106	ALA	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	107	ASP	-	linker	UNP D0LID5
Q	108	ALA	-	linker	UNP D0LID5
Q	109	TRP	-	linker	UNP D0LID5
Q	110	GLU	-	linker	UNP D0LID5
Q	111	GLU	-	linker	UNP D0LID5
Q	112	ASP	-	linker	UNP D0LID5
Q	113	THR	-	linker	UNP D0LID5
Q	114	GLU	-	linker	UNP D0LID5
Q	115	SER	-	linker	UNP D0LID5
R	100	LEU	-	linker	UNP D0LID5
R	101	ASP	-	linker	UNP D0LID5
R	102	ALA	-	linker	UNP D0LID5
R	103	PRO	-	linker	UNP D0LID5
R	104	VAL	-	linker	UNP D0LID5
R	105	VAL	-	linker	UNP D0LID5
R	106	ALA	-	linker	UNP D0LID5
R	107	ASP	-	linker	UNP D0LID5
R	108	ALA	-	linker	UNP D0LID5
R	109	TRP	-	linker	UNP D0LID5
R	110	GLU	-	linker	UNP D0LID5
R	111	GLU	-	linker	UNP D0LID5
R	112	ASP	-	linker	UNP D0LID5
R	113	THR	-	linker	UNP D0LID5
R	114	GLU	-	linker	UNP D0LID5
R	115	SER	-	linker	UNP D0LID5
S	100	LEU	-	linker	UNP D0LID5
S	101	ASP	-	linker	UNP D0LID5
S	102	ALA	-	linker	UNP D0LID5
S	103	PRO	-	linker	UNP D0LID5
S	104	VAL	-	linker	UNP D0LID5
S	105	VAL	-	linker	UNP D0LID5
S	106	ALA	-	linker	UNP D0LID5
S	107	ASP	-	linker	UNP D0LID5
S	108	ALA	-	linker	UNP D0LID5
S	109	TRP	-	linker	UNP D0LID5
S	110	GLU	-	linker	UNP D0LID5
S	111	GLU	-	linker	UNP D0LID5
S	112	ASP	-	linker	UNP D0LID5
S	113	THR	-	linker	UNP D0LID5
S	114	GLU	-	linker	UNP D0LID5
S	115	SER	-	linker	UNP D0LID5
T	100	LEU	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
T	101	ASP	-	linker	UNP D0LID5
T	102	ALA	-	linker	UNP D0LID5
T	103	PRO	-	linker	UNP D0LID5
T	104	VAL	-	linker	UNP D0LID5
T	105	VAL	-	linker	UNP D0LID5
T	106	ALA	-	linker	UNP D0LID5
T	107	ASP	-	linker	UNP D0LID5
T	108	ALA	-	linker	UNP D0LID5
T	109	TRP	-	linker	UNP D0LID5
T	110	GLU	-	linker	UNP D0LID5
T	111	GLU	-	linker	UNP D0LID5
T	112	ASP	-	linker	UNP D0LID5
T	113	THR	-	linker	UNP D0LID5
T	114	GLU	-	linker	UNP D0LID5
T	115	SER	-	linker	UNP D0LID5
U	100	LEU	-	linker	UNP D0LID5
U	101	ASP	-	linker	UNP D0LID5
U	102	ALA	-	linker	UNP D0LID5
U	103	PRO	-	linker	UNP D0LID5
U	104	VAL	-	linker	UNP D0LID5
U	105	VAL	-	linker	UNP D0LID5
U	106	ALA	-	linker	UNP D0LID5
U	107	ASP	-	linker	UNP D0LID5
U	108	ALA	-	linker	UNP D0LID5
U	109	TRP	-	linker	UNP D0LID5
U	110	GLU	-	linker	UNP D0LID5
U	111	GLU	-	linker	UNP D0LID5
U	112	ASP	-	linker	UNP D0LID5
U	113	THR	-	linker	UNP D0LID5
U	114	GLU	-	linker	UNP D0LID5
U	115	SER	-	linker	UNP D0LID5
V	100	LEU	-	linker	UNP D0LID5
V	101	ASP	-	linker	UNP D0LID5
V	102	ALA	-	linker	UNP D0LID5
V	103	PRO	-	linker	UNP D0LID5
V	104	VAL	-	linker	UNP D0LID5
V	105	VAL	-	linker	UNP D0LID5
V	106	ALA	-	linker	UNP D0LID5
V	107	ASP	-	linker	UNP D0LID5
V	108	ALA	-	linker	UNP D0LID5
V	109	TRP	-	linker	UNP D0LID5
V	110	GLU	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
V	111	GLU	-	linker	UNP D0LID5
V	112	ASP	-	linker	UNP D0LID5
V	113	THR	-	linker	UNP D0LID5
V	114	GLU	-	linker	UNP D0LID5
V	115	SER	-	linker	UNP D0LID5
W	100	LEU	-	linker	UNP D0LID5
W	101	ASP	-	linker	UNP D0LID5
W	102	ALA	-	linker	UNP D0LID5
W	103	PRO	-	linker	UNP D0LID5
W	104	VAL	-	linker	UNP D0LID5
W	105	VAL	-	linker	UNP D0LID5
W	106	ALA	-	linker	UNP D0LID5
W	107	ASP	-	linker	UNP D0LID5
W	108	ALA	-	linker	UNP D0LID5
W	109	TRP	-	linker	UNP D0LID5
W	110	GLU	-	linker	UNP D0LID5
W	111	GLU	-	linker	UNP D0LID5
W	112	ASP	-	linker	UNP D0LID5
W	113	THR	-	linker	UNP D0LID5
W	114	GLU	-	linker	UNP D0LID5
W	115	SER	-	linker	UNP D0LID5
X	100	LEU	-	linker	UNP D0LID5
X	101	ASP	-	linker	UNP D0LID5
X	102	ALA	-	linker	UNP D0LID5
X	103	PRO	-	linker	UNP D0LID5
X	104	VAL	-	linker	UNP D0LID5
X	105	VAL	-	linker	UNP D0LID5
X	106	ALA	-	linker	UNP D0LID5
X	107	ASP	-	linker	UNP D0LID5
X	108	ALA	-	linker	UNP D0LID5
X	109	TRP	-	linker	UNP D0LID5
X	110	GLU	-	linker	UNP D0LID5
X	111	GLU	-	linker	UNP D0LID5
X	112	ASP	-	linker	UNP D0LID5
X	113	THR	-	linker	UNP D0LID5
X	114	GLU	-	linker	UNP D0LID5
X	115	SER	-	linker	UNP D0LID5
Y	100	LEU	-	linker	UNP D0LID5
Y	101	ASP	-	linker	UNP D0LID5
Y	102	ALA	-	linker	UNP D0LID5
Y	103	PRO	-	linker	UNP D0LID5
Y	104	VAL	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	105	VAL	-	linker	UNP D0LID5
Y	106	ALA	-	linker	UNP D0LID5
Y	107	ASP	-	linker	UNP D0LID5
Y	108	ALA	-	linker	UNP D0LID5
Y	109	TRP	-	linker	UNP D0LID5
Y	110	GLU	-	linker	UNP D0LID5
Y	111	GLU	-	linker	UNP D0LID5
Y	112	ASP	-	linker	UNP D0LID5
Y	113	THR	-	linker	UNP D0LID5
Y	114	GLU	-	linker	UNP D0LID5
Y	115	SER	-	linker	UNP D0LID5
Z	100	LEU	-	linker	UNP D0LID5
Z	101	ASP	-	linker	UNP D0LID5
Z	102	ALA	-	linker	UNP D0LID5
Z	103	PRO	-	linker	UNP D0LID5
Z	104	VAL	-	linker	UNP D0LID5
Z	105	VAL	-	linker	UNP D0LID5
Z	106	ALA	-	linker	UNP D0LID5
Z	107	ASP	-	linker	UNP D0LID5
Z	108	ALA	-	linker	UNP D0LID5
Z	109	TRP	-	linker	UNP D0LID5
Z	110	GLU	-	linker	UNP D0LID5
Z	111	GLU	-	linker	UNP D0LID5
Z	112	ASP	-	linker	UNP D0LID5
Z	113	THR	-	linker	UNP D0LID5
Z	114	GLU	-	linker	UNP D0LID5
Z	115	SER	-	linker	UNP D0LID5
a	100	LEU	-	linker	UNP D0LID5
a	101	ASP	-	linker	UNP D0LID5
a	102	ALA	-	linker	UNP D0LID5
a	103	PRO	-	linker	UNP D0LID5
a	104	VAL	-	linker	UNP D0LID5
a	105	VAL	-	linker	UNP D0LID5
a	106	ALA	-	linker	UNP D0LID5
a	107	ASP	-	linker	UNP D0LID5
a	108	ALA	-	linker	UNP D0LID5
a	109	TRP	-	linker	UNP D0LID5
a	110	GLU	-	linker	UNP D0LID5
a	111	GLU	-	linker	UNP D0LID5
a	112	ASP	-	linker	UNP D0LID5
a	113	THR	-	linker	UNP D0LID5
a	114	GLU	-	linker	UNP D0LID5

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Chain	Residue	Modelled	Actual	Comment	Reference
a	115	SER	-	linker	UNP D0LID5
b	100	LEU	-	linker	UNP D0LID5
b	101	ASP	-	linker	UNP D0LID5
b	102	ALA	-	linker	UNP D0LID5
b	103	PRO	-	linker	UNP D0LID5
b	104	VAL	-	linker	UNP D0LID5
b	105	VAL	-	linker	UNP D0LID5
b	106	ALA	-	linker	UNP D0LID5
b	107	ASP	-	linker	UNP D0LID5
b	108	ALA	-	linker	UNP D0LID5
b	109	TRP	-	linker	UNP D0LID5
b	110	GLU	-	linker	UNP D0LID5
b	111	GLU	-	linker	UNP D0LID5
b	112	ASP	-	linker	UNP D0LID5
b	113	THR	-	linker	UNP D0LID5
b	114	GLU	-	linker	UNP D0LID5
b	115	SER	-	linker	UNP D0LID5
c	100	LEU	-	linker	UNP D0LID5
c	101	ASP	-	linker	UNP D0LID5
c	102	ALA	-	linker	UNP D0LID5
c	103	PRO	-	linker	UNP D0LID5
c	104	VAL	-	linker	UNP D0LID5
c	105	VAL	-	linker	UNP D0LID5
c	106	ALA	-	linker	UNP D0LID5
c	107	ASP	-	linker	UNP D0LID5
c	108	ALA	-	linker	UNP D0LID5
c	109	TRP	-	linker	UNP D0LID5
c	110	GLU	-	linker	UNP D0LID5
c	111	GLU	-	linker	UNP D0LID5
c	112	ASP	-	linker	UNP D0LID5
c	113	THR	-	linker	UNP D0LID5
c	114	GLU	-	linker	UNP D0LID5
c	115	SER	-	linker	UNP D0LID5
d	100	LEU	-	linker	UNP D0LID5
d	101	ASP	-	linker	UNP D0LID5
d	102	ALA	-	linker	UNP D0LID5
d	103	PRO	-	linker	UNP D0LID5
d	104	VAL	-	linker	UNP D0LID5
d	105	VAL	-	linker	UNP D0LID5
d	106	ALA	-	linker	UNP D0LID5
d	107	ASP	-	linker	UNP D0LID5
d	108	ALA	-	linker	UNP D0LID5

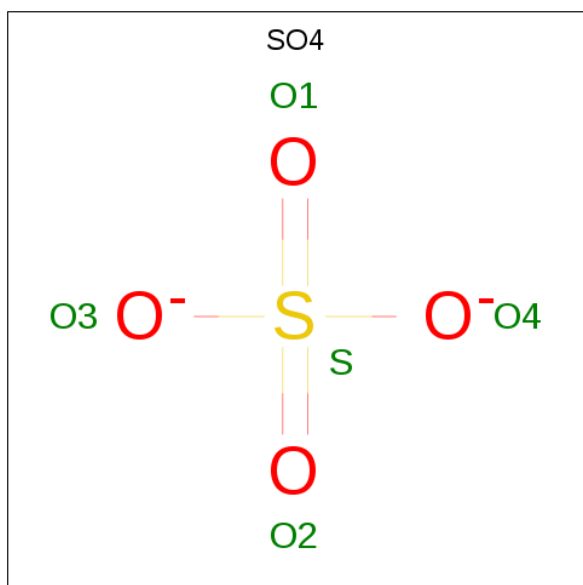
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Chain	Residue	Modelled	Actual	Comment	Reference
d	109	TRP	-	linker	UNP D0LID5
d	110	GLU	-	linker	UNP D0LID5
d	111	GLU	-	linker	UNP D0LID5
d	112	ASP	-	linker	UNP D0LID5
d	113	THR	-	linker	UNP D0LID5
d	114	GLU	-	linker	UNP D0LID5
d	115	SER	-	linker	UNP D0LID5

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	V	1	Total	O	S	0	0
			5	4	1		

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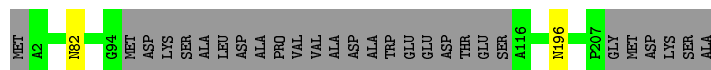
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Y	1	Total	O	S	0	0
			5	4	1		
2	c	1	Total	O	S	0	0
			5	4	1		

### 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.

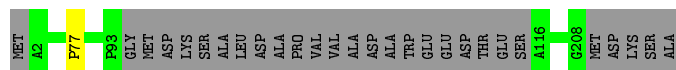
- Molecule 1: BMC-H tandem fusion protein

Chain A: 




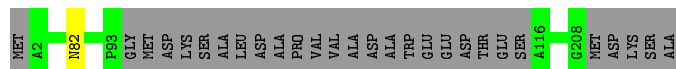
- Molecule 1: BMC-H tandem fusion protein

Chain B: 




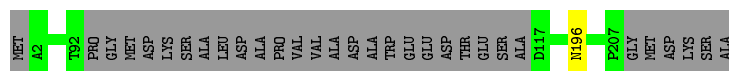
- Molecule 1: BMC-H tandem fusion protein

Chain C: 




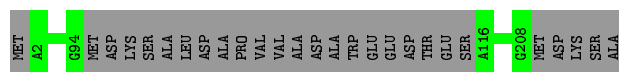
- Molecule 1: BMC-H tandem fusion protein

Chain D: 




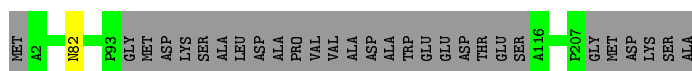
- Molecule 1: BMC-H tandem fusion protein

Chain E: 



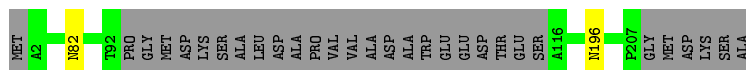
- Molecule 1: BMC-H tandem fusion protein

Chain F: 



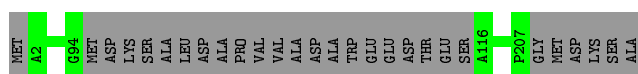
- Molecule 1: BMC-H tandem fusion protein

Chain G: 85% 14%



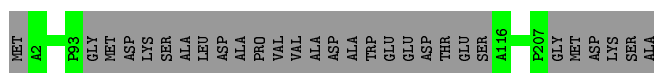
- Molecule 1: BMC-H tandem fusion protein

Chain H: 87% 13%



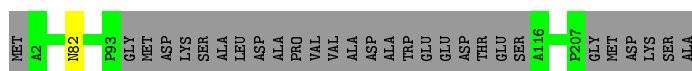
- Molecule 1: BMC-H tandem fusion protein

Chain I: 86% 14%



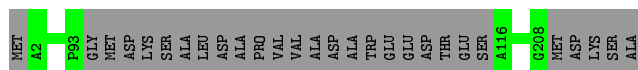
- Molecule 1: BMC-H tandem fusion protein

Chain J: 86% 14%



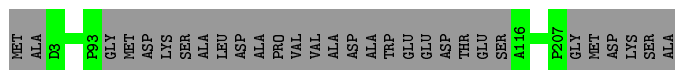
- Molecule 1: BMC-H tandem fusion protein

Chain K: 87% 13%



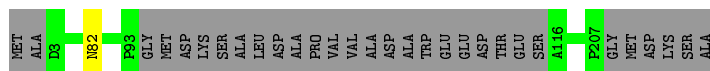
- Molecule 1: BMC-H tandem fusion protein

Chain L: 86% 14%



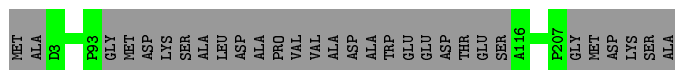
- Molecule 1: BMC-H tandem fusion protein

Chain M: 85% 14%



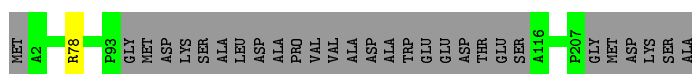
- Molecule 1: BMC-H tandem fusion protein

Chain N: 86% 14%



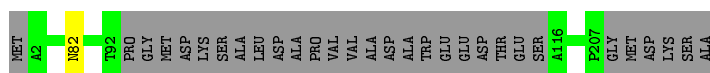
- Molecule 1: BMC-H tandem fusion protein

Chain O: 86% 14%



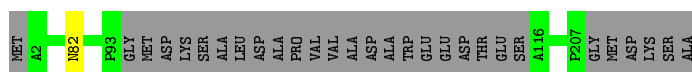
- Molecule 1: BMC-H tandem fusion protein

Chain P: 85% 14%



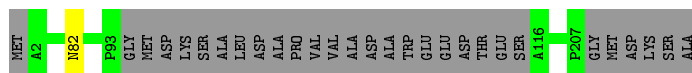
- Molecule 1: BMC-H tandem fusion protein

Chain Q: 86% 14%



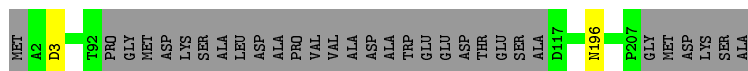
- Molecule 1: BMC-H tandem fusion protein

Chain R: 86% 14%



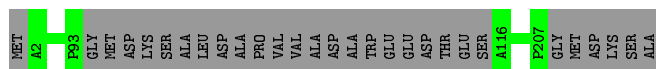
- Molecule 1: BMC-H tandem fusion protein

Chain S: 85% 15%



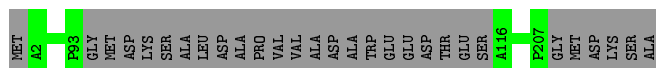
- Molecule 1: BMC-H tandem fusion protein

Chain T: 86% 14%



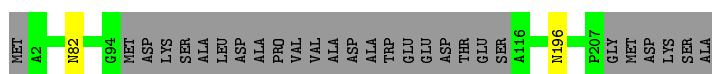
- Molecule 1: BMC-H tandem fusion protein

Chain U: 86% 14%



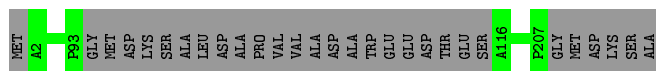
- Molecule 1: BMC-H tandem fusion protein

Chain V: 86% 13%



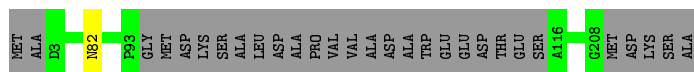
- Molecule 1: BMC-H tandem fusion protein

Chain W: 86% 14%



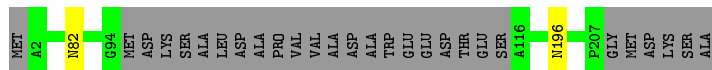
- Molecule 1: BMC-H tandem fusion protein

Chain X: 86% 14%



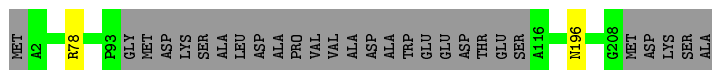
- Molecule 1: BMC-H tandem fusion protein

Chain Y: 86% 13%



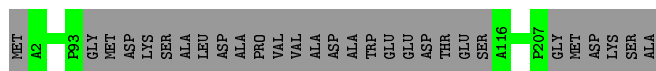
- Molecule 1: BMC-H tandem fusion protein

Chain Z: 86% 13%

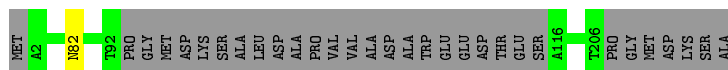
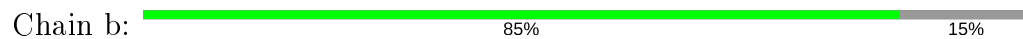


- Molecule 1: BMC-H tandem fusion protein

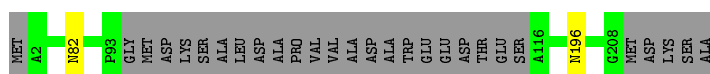
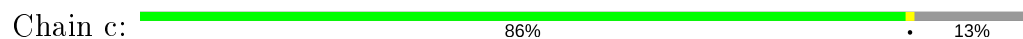
Chain a: 86% 14%



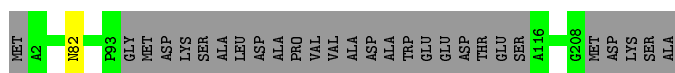
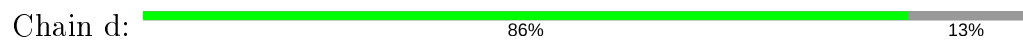
- Molecule 1: BMC-H tandem fusion protein



- Molecule 1: BMC-H tandem fusion protein



- Molecule 1: BMC-H tandem fusion protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	325.51Å 325.51Å 325.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 3.59 49.64 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.64-3.59) 99.9 (49.64-3.59)	Depositor EDS
$R_{merge}$	0.58	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, $R_{free}$	0.171 , 0.210 0.171 , 0.210	Depositor DCC
$R_{free}$ test set	1676 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	117.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	39510	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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

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	0.24	0/1336	0.42	0/1813
1	B	0.24	0/1336	0.41	0/1813
1	C	0.23	0/1336	0.41	0/1813
1	D	0.23	0/1319	0.41	0/1789
1	E	0.24	0/1340	0.42	0/1818
1	F	0.23	0/1332	0.41	0/1808
1	G	0.23	0/1324	0.42	0/1796
1	H	0.24	0/1336	0.41	0/1813
1	I	0.24	0/1332	0.41	0/1808
1	J	0.23	0/1332	0.41	0/1808
1	K	0.24	0/1336	0.41	0/1813
1	L	0.24	0/1327	0.42	0/1801
1	M	0.23	0/1327	0.41	0/1801
1	N	0.23	0/1327	0.42	0/1801
1	O	0.24	0/1332	0.42	0/1808
1	P	0.23	0/1324	0.41	0/1796
1	Q	0.24	0/1332	0.41	0/1808
1	R	0.23	0/1332	0.41	0/1808
1	S	0.24	0/1319	0.41	0/1789
1	T	0.23	0/1332	0.41	0/1808
1	U	0.23	0/1332	0.41	0/1808
1	V	0.23	0/1336	0.41	0/1813
1	W	0.24	0/1332	0.41	0/1808
1	X	0.23	0/1331	0.41	0/1806
1	Y	0.24	0/1336	0.41	0/1813
1	Z	0.23	0/1336	0.41	0/1813
1	a	0.23	0/1332	0.41	0/1808
1	b	0.23	0/1316	0.42	0/1784
1	c	0.24	0/1336	0.41	0/1813
1	d	0.23	0/1336	0.41	0/1813
All	All	0.23	0/39934	0.41	0/54191

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	181/213 (85%)	176 (97%)	5 (3%)	0	100	100
1	B	181/213 (85%)	173 (96%)	7 (4%)	1 (1%)	25	64
1	C	181/213 (85%)	172 (95%)	9 (5%)	0	100	100
1	D	178/213 (84%)	171 (96%)	7 (4%)	0	100	100
1	E	182/213 (85%)	177 (97%)	5 (3%)	0	100	100
1	F	180/213 (84%)	172 (96%)	8 (4%)	0	100	100
1	G	179/213 (84%)	171 (96%)	8 (4%)	0	100	100
1	H	181/213 (85%)	173 (96%)	8 (4%)	0	100	100
1	I	180/213 (84%)	172 (96%)	8 (4%)	0	100	100
1	J	180/213 (84%)	175 (97%)	5 (3%)	0	100	100
1	K	181/213 (85%)	174 (96%)	7 (4%)	0	100	100
1	L	179/213 (84%)	173 (97%)	6 (3%)	0	100	100
1	M	179/213 (84%)	172 (96%)	7 (4%)	0	100	100
1	N	179/213 (84%)	172 (96%)	7 (4%)	0	100	100
1	O	180/213 (84%)	172 (96%)	8 (4%)	0	100	100
1	P	179/213 (84%)	172 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	180/213 (84%)	172 (96%)	8 (4%)	0	100	100
1	R	180/213 (84%)	173 (96%)	7 (4%)	0	100	100
1	S	178/213 (84%)	172 (97%)	6 (3%)	0	100	100
1	T	180/213 (84%)	174 (97%)	6 (3%)	0	100	100
1	U	180/213 (84%)	173 (96%)	7 (4%)	0	100	100
1	V	181/213 (85%)	176 (97%)	5 (3%)	0	100	100
1	W	180/213 (84%)	172 (96%)	8 (4%)	0	100	100
1	X	180/213 (84%)	171 (95%)	9 (5%)	0	100	100
1	Y	181/213 (85%)	175 (97%)	6 (3%)	0	100	100
1	Z	181/213 (85%)	172 (95%)	9 (5%)	0	100	100
1	a	180/213 (84%)	174 (97%)	6 (3%)	0	100	100
1	b	178/213 (84%)	171 (96%)	7 (4%)	0	100	100
1	c	181/213 (85%)	172 (95%)	9 (5%)	0	100	100
1	d	181/213 (85%)	173 (96%)	8 (4%)	0	100	100
All	All	5401/6390 (84%)	5187 (96%)	213 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	PRO

### 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	126/148 (85%)	124 (98%)	2 (2%)	62	83
1	B	126/148 (85%)	126 (100%)	0	100	100
1	C	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	D	125/148 (84%)	124 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	126/148 (85%)	126 (100%)	0	100	100
1	F	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	G	125/148 (84%)	123 (98%)	2 (2%)	62	83
1	H	126/148 (85%)	126 (100%)	0	100	100
1	I	126/148 (85%)	126 (100%)	0	100	100
1	J	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	K	126/148 (85%)	126 (100%)	0	100	100
1	L	126/148 (85%)	126 (100%)	0	100	100
1	M	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	N	126/148 (85%)	126 (100%)	0	100	100
1	O	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	P	125/148 (84%)	124 (99%)	1 (1%)	81	91
1	Q	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	R	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	S	125/148 (84%)	123 (98%)	2 (2%)	62	83
1	T	126/148 (85%)	126 (100%)	0	100	100
1	U	126/148 (85%)	126 (100%)	0	100	100
1	V	126/148 (85%)	124 (98%)	2 (2%)	62	83
1	W	126/148 (85%)	126 (100%)	0	100	100
1	X	126/148 (85%)	125 (99%)	1 (1%)	81	91
1	Y	126/148 (85%)	124 (98%)	2 (2%)	62	83
1	Z	126/148 (85%)	124 (98%)	2 (2%)	62	83
1	a	126/148 (85%)	126 (100%)	0	100	100
1	b	124/148 (84%)	123 (99%)	1 (1%)	81	91
1	c	126/148 (85%)	124 (98%)	2 (2%)	62	83
1	d	126/148 (85%)	125 (99%)	1 (1%)	81	91
All	All	3774/4440 (85%)	3748 (99%)	26 (1%)	84	93

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	196	ASN

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Mol	Chain	Res	Type
1	C	82	ASN
1	D	196	ASN
1	F	82	ASN
1	G	82	ASN
1	G	196	ASN
1	J	82	ASN
1	M	82	ASN
1	O	78	ARG
1	P	82	ASN
1	Q	82	ASN
1	R	82	ASN
1	S	3	ASP
1	S	196	ASN
1	V	82	ASN
1	V	196	ASN
1	X	82	ASN
1	Y	82	ASN
1	Y	196	ASN
1	Z	78	ARG
1	Z	196	ASN
1	b	82	ASN
1	c	82	ASN
1	c	196	ASN
1	d	82	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

10 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	SO4	M	301	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	c	301	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	G	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	Y	301	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	S	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	V	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	P	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	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.

No monomer is involved in short contacts.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	185/213 (86%)	-0.25	0 100 100	85, 111, 138, 159	0
1	B	185/213 (86%)	-0.32	0 100 100	86, 109, 135, 153	0
1	C	185/213 (86%)	-0.32	0 100 100	83, 109, 143, 167	0
1	D	182/213 (85%)	-0.31	0 100 100	86, 110, 139, 166	0
1	E	186/213 (87%)	-0.45	0 100 100	85, 107, 134, 152	0
1	F	184/213 (86%)	-0.29	0 100 100	85, 109, 138, 171	0
1	G	183/213 (85%)	-0.31	0 100 100	88, 112, 141, 166	0
1	H	185/213 (86%)	-0.36	0 100 100	90, 112, 138, 156	0
1	I	184/213 (86%)	-0.34	0 100 100	80, 110, 140, 169	0
1	J	184/213 (86%)	-0.30	0 100 100	91, 114, 145, 165	0
1	K	185/213 (86%)	-0.32	0 100 100	87, 111, 140, 153	0
1	L	183/213 (85%)	-0.47	0 100 100	90, 113, 140, 175	0
1	M	183/213 (85%)	-0.33	0 100 100	87, 109, 140, 165	0
1	N	183/213 (85%)	-0.35	0 100 100	86, 109, 134, 150	0
1	O	184/213 (86%)	-0.40	0 100 100	82, 109, 143, 159	0
1	P	183/213 (85%)	-0.32	0 100 100	91, 112, 147, 165	0
1	Q	184/213 (86%)	-0.36	0 100 100	84, 110, 140, 152	0
1	R	184/213 (86%)	-0.37	0 100 100	84, 109, 141, 170	0
1	S	182/213 (85%)	-0.35	0 100 100	89, 112, 143, 161	0
1	T	184/213 (86%)	-0.41	0 100 100	84, 110, 135, 154	0
1	U	184/213 (86%)	-0.40	0 100 100	85, 110, 143, 161	0
1	V	185/213 (86%)	-0.26	0 100 100	86, 109, 144, 176	0
1	W	184/213 (86%)	-0.35	0 100 100	84, 105, 133, 152	0
1	X	184/213 (86%)	-0.43	0 100 100	87, 108, 134, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9	
1	Y	185/213 (86%)	-0.21	0	100 100	86, 111, 143, 166	0
1	Z	185/213 (86%)	-0.27	0	100 100	85, 109, 136, 151	0
1	a	184/213 (86%)	-0.26	0	100 100	84, 109, 144, 167	0
1	b	182/213 (85%)	-0.31	0	100 100	90, 113, 144, 161	0
1	c	185/213 (86%)	-0.37	0	100 100	91, 111, 140, 155	0
1	d	185/213 (86%)	-0.34	0	100 100	85, 110, 143, 172	0
All	All	5521/6390 (86%)	-0.34	0	100 100	80, 110, 141, 176	0

There are no RSRZ outliers to report.

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	D	301	5/5	0.92	0.14	88,115,125,129	0
2	SO4	S	301	5/5	0.93	0.18	99,100,120,125	0
2	SO4	P	301	5/5	0.93	0.20	104,107,126,137	0
2	SO4	L	301	5/5	0.93	0.19	107,112,123,128	0
2	SO4	G	301	5/5	0.94	0.17	91,103,119,125	0
2	SO4	M	301	5/5	0.94	0.12	93,106,117,127	0
2	SO4	c	301	5/5	0.94	0.18	106,112,117,120	0
2	SO4	A	301	5/5	0.94	0.13	101,106,125,127	0
2	SO4	Y	301	5/5	0.95	0.15	78,108,123,125	0
2	SO4	V	301	5/5	0.96	0.14	101,107,123,135	0



## 6.5 Other polymers

There are no such residues in this entry.