



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 10:57 PM BST

PDB ID : 3ANZ
Title : Crystal Structure of alpha-hemolysin
Authors : Yamashita, K.; Kawauchi, H.; Tanaka, Y.; Yao, M.; Tanaka, I.
Deposited on : 2010-09-16
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

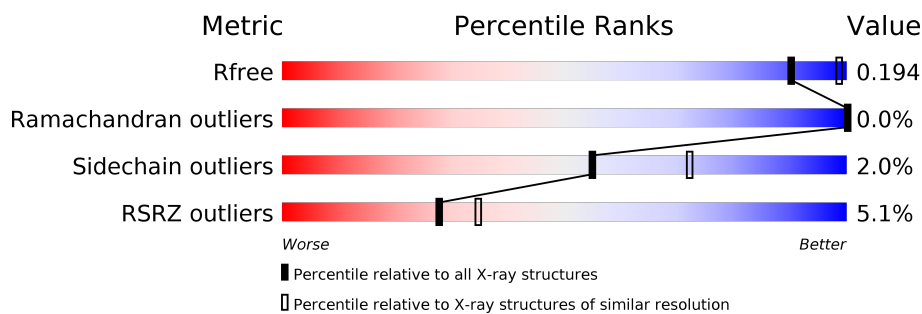
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	302	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
1	B	302	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
1	C	302	<div> <div>5%</div> <div>96%</div> <div>..</div> </div>
1	D	302	<div> <div>5%</div> <div>95%</div> <div>..</div> </div>
1	E	302	<div> <div>10%</div> <div>94%</div> <div>..</div> </div>
1	F	302	<div> <div>8%</div> <div>95%</div> <div>..</div> </div>
1	G	302	<div> <div>6%</div> <div>96%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	302	
1	I	302	
1	J	302	
1	K	302	
1	L	302	
1	M	302	
1	N	302	
1	O	302	
1	P	302	
1	Q	302	
1	R	302	
1	S	302	
1	T	302	
1	U	302	
1	V	302	
1	W	302	
1	X	302	
1	Y	302	
1	Z	302	
1	a	302	
1	b	302	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	Q	303	-	-	-	X
2	MPD	X	304	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	S	304	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 68607 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 Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	B	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	C	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	D	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	E	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	F	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	G	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	H	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	I	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	J	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	K	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	L	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	M	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	N	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	O	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	P	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	R	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	S	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	T	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	U	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	V	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			
1	W	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	X	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	Y	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	Z	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	a	294	Total	C	N	O	S	0	0	0
			2353	1479	402	465	7			
1	b	295	Total	C	N	O	S	0	0	0
			2362	1484	403	468	7			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q99UU6
A	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
A	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
A	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
A	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	0	MET	-	EXPRESSION TAG	UNP Q99UU6
B	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
B	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
B	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	298	HIS	-	EXPRESSION TAG	UNP Q99UU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
B	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	0	MET	-	EXPRESSION TAG	UNP Q99UU6
C	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
C	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
C	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
C	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	0	MET	-	EXPRESSION TAG	UNP Q99UU6
D	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
D	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
D	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
D	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	0	MET	-	EXPRESSION TAG	UNP Q99UU6
E	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
E	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
E	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
E	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	0	MET	-	EXPRESSION TAG	UNP Q99UU6
F	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
F	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
F	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
F	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	0	MET	-	EXPRESSION TAG	UNP Q99UU6
G	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
G	295	GLU	-	EXPRESSION TAG	UNP Q99UU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
G	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	0	MET	-	EXPRESSION TAG	UNP Q99UU6
H	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
H	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
H	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
H	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	0	MET	-	EXPRESSION TAG	UNP Q99UU6
I	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
I	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
I	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
I	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	0	MET	-	EXPRESSION TAG	UNP Q99UU6
J	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
J	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
J	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
J	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	0	MET	-	EXPRESSION TAG	UNP Q99UU6
K	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
K	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
K	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
K	301	HIS	-	EXPRESSION TAG	UNP Q99UU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	EXPRESSION TAG	UNP Q99UU6
L	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
L	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
L	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
L	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	0	MET	-	EXPRESSION TAG	UNP Q99UU6
M	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
M	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
M	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
M	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	0	MET	-	EXPRESSION TAG	UNP Q99UU6
N	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
N	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
N	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
N	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	0	MET	-	EXPRESSION TAG	UNP Q99UU6
O	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
O	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
O	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
O	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	0	MET	-	EXPRESSION TAG	UNP Q99UU6
P	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
P	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
P	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	298	HIS	-	EXPRESSION TAG	UNP Q99UU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
P	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	0	MET	-	EXPRESSION TAG	UNP Q99UU6
Q	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
Q	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
Q	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
Q	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	0	MET	-	EXPRESSION TAG	UNP Q99UU6
R	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
R	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
R	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
R	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	0	MET	-	EXPRESSION TAG	UNP Q99UU6
S	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
S	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
S	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
S	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	0	MET	-	EXPRESSION TAG	UNP Q99UU6
T	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
T	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
T	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
T	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	0	MET	-	EXPRESSION TAG	UNP Q99UU6
U	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
U	295	GLU	-	EXPRESSION TAG	UNP Q99UU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
U	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	0	MET	-	EXPRESSION TAG	UNP Q99UU6
V	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
V	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
V	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
V	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	0	MET	-	EXPRESSION TAG	UNP Q99UU6
W	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
W	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
W	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
W	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	0	MET	-	EXPRESSION TAG	UNP Q99UU6
X	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
X	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
X	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
X	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	0	MET	-	EXPRESSION TAG	UNP Q99UU6
Y	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
Y	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
Y	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
Y	301	HIS	-	EXPRESSION TAG	UNP Q99UU6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Z	0	MET	-	EXPRESSION TAG	UNP Q99UU6
Z	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
Z	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
Z	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
Z	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	0	MET	-	EXPRESSION TAG	UNP Q99UU6
a	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
a	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
a	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
a	301	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	0	MET	-	EXPRESSION TAG	UNP Q99UU6
b	294	LEU	-	EXPRESSION TAG	UNP Q99UU6
b	295	GLU	-	EXPRESSION TAG	UNP Q99UU6
b	296	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	297	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	298	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	299	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	300	HIS	-	EXPRESSION TAG	UNP Q99UU6
b	301	HIS	-	EXPRESSION TAG	UNP Q99UU6

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		
2	G	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

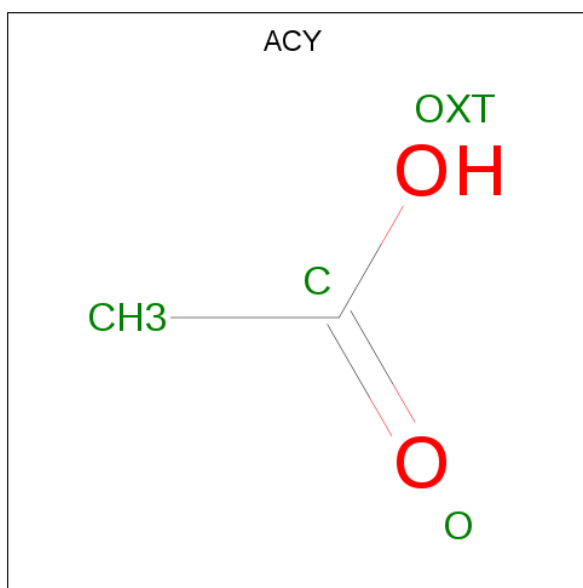
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			8	6	2		
2	H	1	Total	C	O	0	0
			8	6	2		
2	I	1	Total	C	O	0	0
			8	6	2		
2	I	1	Total	C	O	0	0
			8	6	2		
2	J	1	Total	C	O	0	0
			8	6	2		
2	J	1	Total	C	O	0	0
			8	6	2		
2	K	1	Total	C	O	0	0
			8	6	2		
2	K	1	Total	C	O	0	0
			8	6	2		
2	L	1	Total	C	O	0	0
			8	6	2		
2	L	1	Total	C	O	0	0
			8	6	2		
2	M	1	Total	C	O	0	0
			8	6	2		
2	M	1	Total	C	O	0	0
			8	6	2		
2	N	1	Total	C	O	0	0
			8	6	2		
2	N	1	Total	C	O	0	0
			8	6	2		
2	O	1	Total	C	O	0	0
			8	6	2		
2	O	1	Total	C	O	0	0
			8	6	2		
2	P	1	Total	C	O	0	0
			8	6	2		
2	P	1	Total	C	O	0	0
			8	6	2		
2	Q	1	Total	C	O	0	0
			8	6	2		
2	Q	1	Total	C	O	0	0
			8	6	2		
2	R	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	R	1	Total	C	O	0	0
			8	6	2		
2	S	1	Total	C	O	0	0
			8	6	2		
2	S	1	Total	C	O	0	0
			8	6	2		
2	T	1	Total	C	O	0	0
			8	6	2		
2	T	1	Total	C	O	0	0
			8	6	2		
2	U	1	Total	C	O	0	0
			8	6	2		
2	U	1	Total	C	O	0	0
			8	6	2		
2	V	1	Total	C	O	0	0
			8	6	2		
2	V	1	Total	C	O	0	0
			8	6	2		
2	W	1	Total	C	O	0	0
			8	6	2		
2	W	1	Total	C	O	0	0
			8	6	2		
2	X	1	Total	C	O	0	0
			8	6	2		
2	X	1	Total	C	O	0	0
			8	6	2		
2	X	1	Total	C	O	0	0
			8	6	2		
2	Y	1	Total	C	O	0	0
			8	6	2		
2	Y	1	Total	C	O	0	0
			8	6	2		
2	Z	1	Total	C	O	0	0
			8	6	2		
2	a	1	Total	C	O	0	0
			8	6	2		
2	a	1	Total	C	O	0	0
			8	6	2		
2	b	1	Total	C	O	0	0
			8	6	2		
2	b	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	P	1	Total C O 4 2 2	0	0
3	Q	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	S	1	Total C O 4 2 2	0	0
3	T	1	Total C O 4 2 2	0	0
3	V	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	X	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	Z	1	Total C O 4 2 2	0	0
3	a	1	Total C O 4 2 2	0	0
3	b	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	94	Total O 94 94	0	0
4	B	79	Total O 79 79	0	0
4	C	73	Total O 73 73	0	0
4	D	66	Total O 66 66	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	54	Total O 54 54	0	0
4	F	46	Total O 46 46	0	0
4	G	70	Total O 70 70	0	0
4	H	89	Total O 89 89	0	0
4	I	87	Total O 87 87	0	0
4	J	86	Total O 86 86	0	0
4	K	97	Total O 97 97	0	0
4	L	71	Total O 71 71	0	0
4	M	61	Total O 61 61	0	0
4	N	73	Total O 73 73	0	0
4	O	91	Total O 91 91	0	0
4	P	73	Total O 73 73	0	0
4	Q	61	Total O 61 61	0	0
4	R	73	Total O 73 73	0	0
4	S	69	Total O 69 69	0	0
4	T	82	Total O 82 82	0	0
4	U	85	Total O 85 85	0	0
4	V	82	Total O 82 82	0	0
4	W	50	Total O 50 50	0	0
4	X	46	Total O 46 46	0	0
4	Y	53	Total O 53 53	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	82	Total 82	O 82	0	0
4	a	99	Total 99	O 99	0	0
4	b	72	Total 72	O 72	0	0

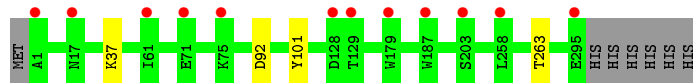
3 Residue-property plots [i](#)

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.

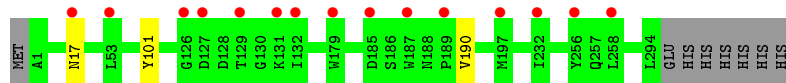
- Molecule 1: Alpha-hemolysin



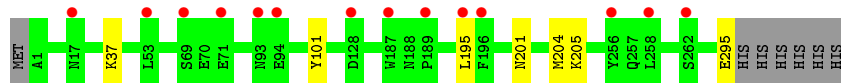
- Molecule 1: Alpha-hemolysin



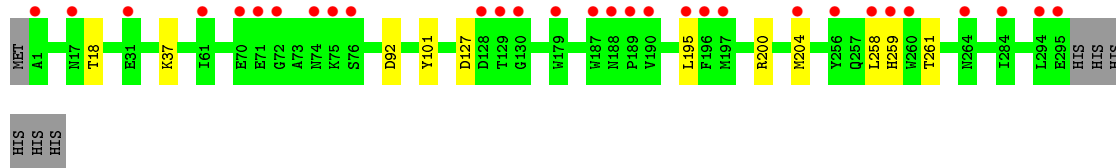
- Molecule 1: Alpha-hemolysin



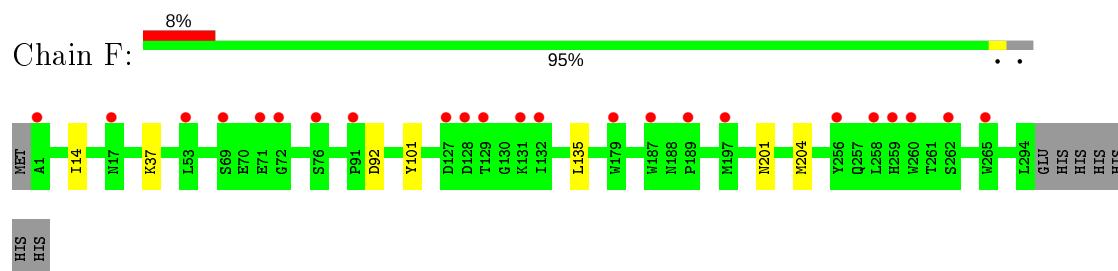
- Molecule 1: Alpha-hemolysin



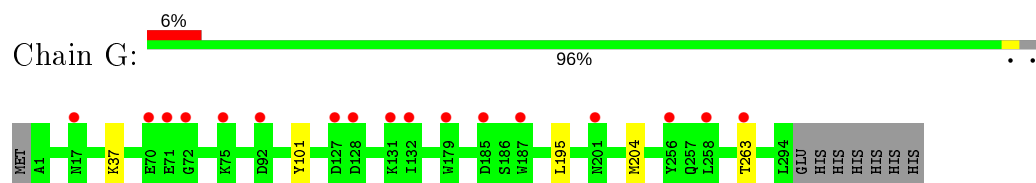
- Molecule 1: Alpha-hemolysin



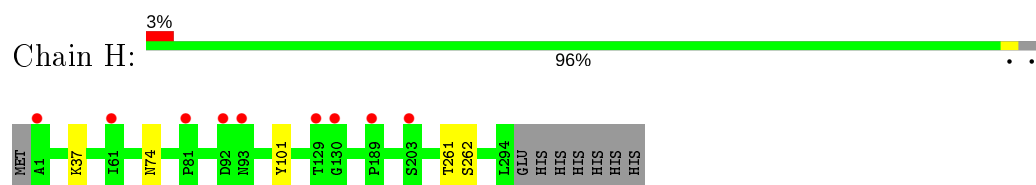
● Molecule 1: Alpha-hemolysin



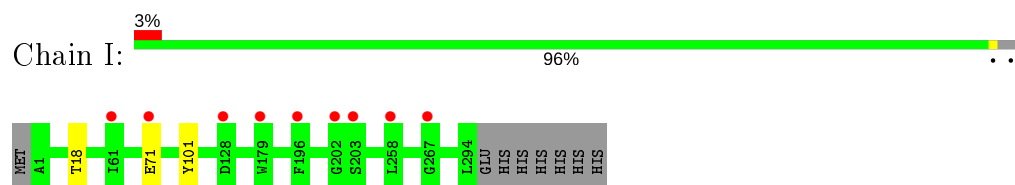
● Molecule 1: Alpha-hemolysin



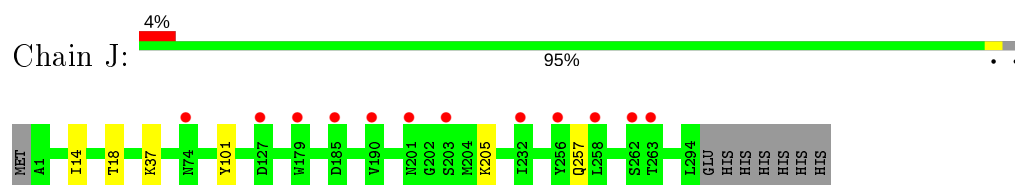
● Molecule 1: Alpha-hemolysin



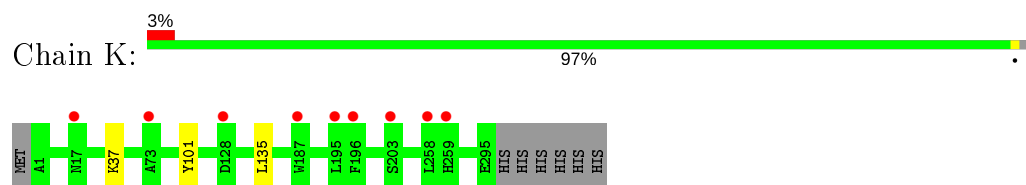
● Molecule 1: Alpha-hemolysin



● Molecule 1: Alpha-hemolysin

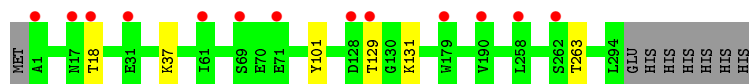


● Molecule 1: Alpha-hemolysin

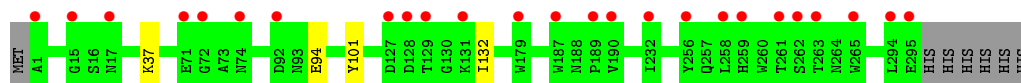


● Molecule 1: Alpha-hemolysin

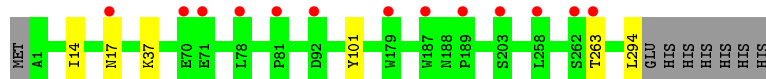




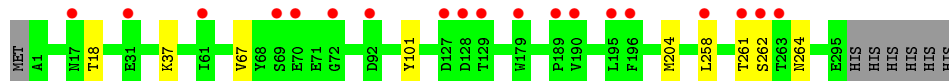
- Molecule 1: Alpha-hemolysin



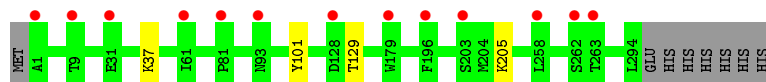
- Molecule 1: Alpha-hemolysin



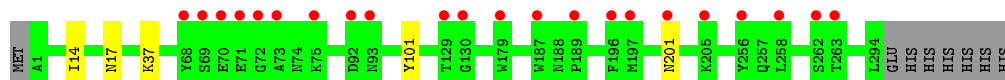
- Molecule 1: Alpha-hemolysin



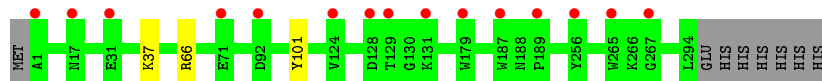
- Molecule 1: Alpha-hemolysin



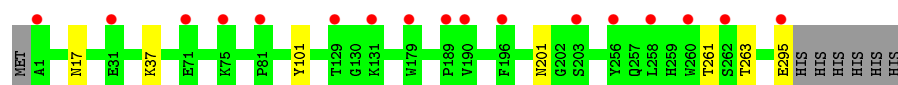
- Molecule 1: Alpha-hemolysin



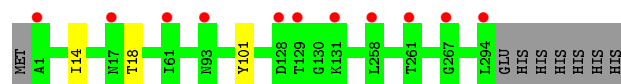
- Molecule 1: Alpha-hemolysin



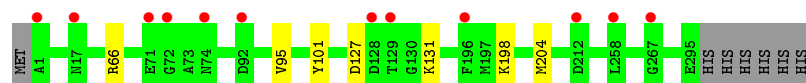
- Molecule 1: Alpha-hemolysin



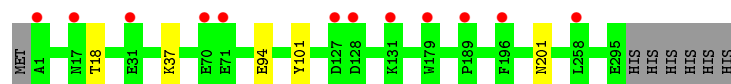
- Molecule 1: Alpha-hemolysin



- Molecule 1: Alpha-hemolysin



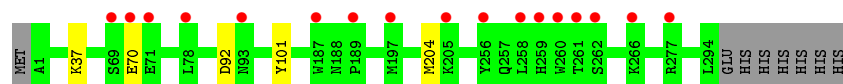
- Molecule 1: Alpha-hemolysin



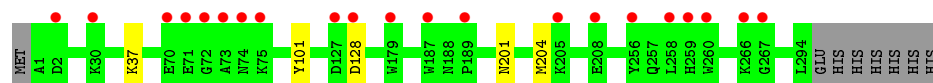
- Molecule 1: Alpha-hemolysin



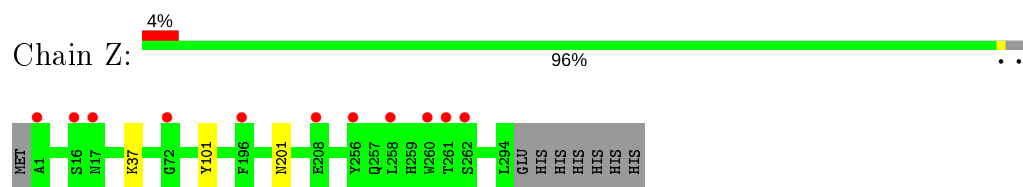
- Molecule 1: Alpha-hemolysin



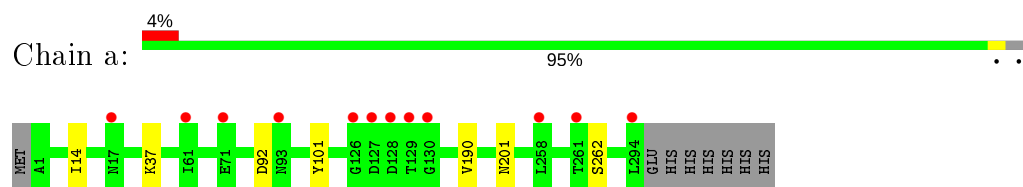
- Molecule 1: Alpha-hemolysin



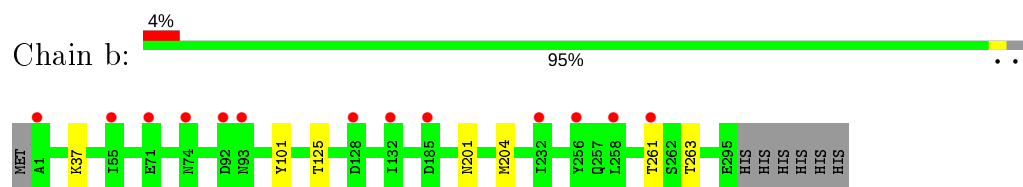
• Molecule 1: Alpha-hemolysin



• Molecule 1: Alpha-hemolysin



• Molecule 1: Alpha-hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.82Å 293.88Å 170.54Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.98-2.30) 98.0 (19.98-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.30Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.193 , 0.226 0.195 , 0.194	Depositor DCC
R_{free} test set	31076 reflections (7.15%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	68607	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3976e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: ACY, MPD

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	0.33	0/2414	0.50	1/3267 (0.0%)
1	B	0.32	0/2414	0.47	0/3267
1	C	0.32	0/2405	0.48	0/3255
1	D	0.32	0/2414	0.47	0/3267
1	E	0.32	0/2414	0.47	0/3267
1	F	0.31	0/2405	0.47	0/3255
1	G	0.32	0/2405	0.48	0/3255
1	H	0.33	0/2405	0.50	1/3255 (0.0%)
1	I	0.32	0/2405	0.48	0/3255
1	J	0.33	0/2405	0.47	0/3255
1	K	0.34	0/2414	0.48	0/3267
1	L	0.34	0/2405	0.48	0/3255
1	M	0.32	0/2414	0.47	0/3267
1	N	0.32	0/2405	0.47	0/3255
1	O	0.33	0/2414	0.47	0/3267
1	P	0.32	0/2405	0.48	0/3255
1	Q	0.32	0/2405	0.46	0/3255
1	R	0.33	0/2405	0.48	0/3255
1	S	0.32	0/2414	0.47	0/3267
1	T	0.33	0/2405	0.48	0/3255
1	U	0.32	0/2414	0.47	0/3267
1	V	0.32	0/2414	0.48	0/3267
1	W	0.32	0/2405	0.46	0/3255
1	X	0.31	0/2405	0.46	0/3255
1	Y	0.31	0/2405	0.47	0/3255
1	Z	0.32	0/2405	0.47	0/3255
1	a	0.33	0/2405	0.48	0/3255
1	b	0.33	0/2414	0.48	0/3267
All	All	0.32	0/67439	0.48	2/91272 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	H	261	THR	N-CA-C	-5.25	96.82	111.00
1	A	261	THR	N-CA-C	-5.19	96.98	111.00

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	293/302 (97%)	280 (96%)	13 (4%)	0	100	100
1	B	293/302 (97%)	278 (95%)	15 (5%)	0	100	100
1	C	292/302 (97%)	282 (97%)	10 (3%)	0	100	100
1	D	293/302 (97%)	282 (96%)	11 (4%)	0	100	100
1	E	293/302 (97%)	275 (94%)	18 (6%)	0	100	100
1	F	292/302 (97%)	280 (96%)	12 (4%)	0	100	100
1	G	292/302 (97%)	279 (96%)	13 (4%)	0	100	100
1	H	292/302 (97%)	278 (95%)	13 (4%)	1 (0%)	41	50
1	I	292/302 (97%)	280 (96%)	12 (4%)	0	100	100
1	J	292/302 (97%)	278 (95%)	14 (5%)	0	100	100
1	K	293/302 (97%)	284 (97%)	9 (3%)	0	100	100
1	L	292/302 (97%)	277 (95%)	15 (5%)	0	100	100
1	M	293/302 (97%)	282 (96%)	11 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	292/302 (97%)	281 (96%)	11 (4%)	0	100	100
1	O	293/302 (97%)	278 (95%)	14 (5%)	1 (0%)	41	50
1	P	292/302 (97%)	281 (96%)	11 (4%)	0	100	100
1	Q	292/302 (97%)	282 (97%)	10 (3%)	0	100	100
1	R	292/302 (97%)	279 (96%)	13 (4%)	0	100	100
1	S	293/302 (97%)	280 (96%)	13 (4%)	0	100	100
1	T	292/302 (97%)	276 (94%)	16 (6%)	0	100	100
1	U	293/302 (97%)	283 (97%)	10 (3%)	0	100	100
1	V	293/302 (97%)	282 (96%)	11 (4%)	0	100	100
1	W	292/302 (97%)	279 (96%)	13 (4%)	0	100	100
1	X	292/302 (97%)	281 (96%)	11 (4%)	0	100	100
1	Y	292/302 (97%)	277 (95%)	15 (5%)	0	100	100
1	Z	292/302 (97%)	280 (96%)	12 (4%)	0	100	100
1	a	292/302 (97%)	279 (96%)	12 (4%)	1 (0%)	41	50
1	b	293/302 (97%)	282 (96%)	11 (4%)	0	100	100
All	All	8187/8456 (97%)	7835 (96%)	349 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	262	SER
1	a	262	SER
1	H	262	SER

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	261/268 (97%)	257 (98%)	4 (2%)	65	79
1	B	261/268 (97%)	257 (98%)	4 (2%)	65	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	260/268 (97%)	257 (99%)	3 (1%)	71	84
1	D	261/268 (97%)	254 (97%)	7 (3%)	44	61
1	E	261/268 (97%)	250 (96%)	11 (4%)	30	42
1	F	260/268 (97%)	253 (97%)	7 (3%)	44	61
1	G	260/268 (97%)	255 (98%)	5 (2%)	57	73
1	H	260/268 (97%)	257 (99%)	3 (1%)	71	84
1	I	260/268 (97%)	257 (99%)	3 (1%)	71	84
1	J	260/268 (97%)	254 (98%)	6 (2%)	50	67
1	K	261/268 (97%)	258 (99%)	3 (1%)	73	86
1	L	260/268 (97%)	254 (98%)	6 (2%)	50	67
1	M	261/268 (97%)	257 (98%)	4 (2%)	65	79
1	N	260/268 (97%)	254 (98%)	6 (2%)	50	67
1	O	261/268 (97%)	253 (97%)	8 (3%)	40	55
1	P	260/268 (97%)	256 (98%)	4 (2%)	65	79
1	Q	260/268 (97%)	255 (98%)	5 (2%)	57	73
1	R	260/268 (97%)	257 (99%)	3 (1%)	71	84
1	S	261/268 (97%)	254 (97%)	7 (3%)	44	61
1	T	260/268 (97%)	257 (99%)	3 (1%)	71	84
1	U	261/268 (97%)	254 (97%)	7 (3%)	44	61
1	V	261/268 (97%)	256 (98%)	5 (2%)	57	73
1	W	260/268 (97%)	255 (98%)	5 (2%)	57	73
1	X	260/268 (97%)	255 (98%)	5 (2%)	57	73
1	Y	260/268 (97%)	255 (98%)	5 (2%)	57	73
1	Z	260/268 (97%)	257 (99%)	3 (1%)	71	84
1	a	260/268 (97%)	254 (98%)	6 (2%)	50	67
1	b	261/268 (97%)	254 (97%)	7 (3%)	44	61
All	All	7291/7504 (97%)	7146 (98%)	145 (2%)	55	72

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	132	ILE
1	P	101	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	92	ASP
1	N	17	ASN
1	O	37	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	C	177	GLN
1	J	97	GLN
1	O	264	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

84 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	MPD	H	303	-	7,7,7	0.25	0	9,10,10	0.44	0
3	ACY	P	304	-	1,3,3	1.55	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	Q	303	-	7,7,7	0.31	0	9,10,10	0.40	0
2	MPD	M	302	-	7,7,7	0.26	0	9,10,10	0.27	0
3	ACY	T	304	-	1,3,3	1.61	0	0,3,3	0.00	-
2	MPD	a	303	-	7,7,7	0.27	0	9,10,10	0.65	0
2	MPD	I	302	-	7,7,7	0.28	0	9,10,10	0.29	0
3	ACY	A	305	-	1,3,3	1.66	0	0,3,3	0.00	-
2	MPD	K	303	-	7,7,7	0.32	0	9,10,10	0.65	0
2	MPD	E	303	-	7,7,7	0.35	0	9,10,10	0.57	0
2	MPD	A	302	-	7,7,7	0.27	0	9,10,10	0.89	0
3	ACY	F	304	-	1,3,3	1.59	0	0,3,3	0.00	-
2	MPD	Y	302	-	7,7,7	0.27	0	9,10,10	0.44	0
3	ACY	H	304	-	1,3,3	1.62	0	0,3,3	0.00	-
3	ACY	X	305	-	1,3,3	1.46	0	0,3,3	0.00	-
2	MPD	F	303	-	7,7,7	0.21	0	9,10,10	0.48	0
2	MPD	U	303	-	7,7,7	0.36	0	9,10,10	0.49	0
3	ACY	O	304	-	1,3,3	1.28	0	0,3,3	0.00	-
3	ACY	E	304	-	1,3,3	1.46	0	0,3,3	0.00	-
2	MPD	H	302	-	7,7,7	0.27	0	9,10,10	0.49	0
2	MPD	M	303	-	7,7,7	0.34	0	9,10,10	0.56	0
2	MPD	F	302	-	7,7,7	0.29	0	9,10,10	0.36	0
3	ACY	M	304	-	1,3,3	1.55	0	0,3,3	0.00	-
2	MPD	I	303	-	7,7,7	0.30	0	9,10,10	0.47	0
3	ACY	K	304	-	1,3,3	1.46	0	0,3,3	0.00	-
3	ACY	H	305	-	1,3,3	1.61	0	0,3,3	0.00	-
3	ACY	K	305	-	1,3,3	1.17	0	0,3,3	0.00	-
2	MPD	a	302	-	7,7,7	0.27	0	9,10,10	0.37	0
2	MPD	A	303	-	7,7,7	0.33	0	9,10,10	0.63	0
3	ACY	S	304	-	1,3,3	1.33	0	0,3,3	0.00	-
3	ACY	A	304	-	1,3,3	1.67	0	0,3,3	0.00	-
2	MPD	T	302	-	7,7,7	0.31	0	9,10,10	0.26	0
2	MPD	S	302	-	7,7,7	0.32	0	9,10,10	0.57	0
2	MPD	P	302	-	7,7,7	0.24	0	9,10,10	0.25	0
2	MPD	U	302	-	7,7,7	0.30	0	9,10,10	0.33	0
2	MPD	Z	302	-	7,7,7	0.28	0	9,10,10	0.44	0
2	MPD	W	303	-	7,7,7	0.32	0	9,10,10	0.50	0
2	MPD	b	303	-	7,7,7	0.33	0	9,10,10	0.46	0
3	ACY	V	304	-	1,3,3	1.60	0	0,3,3	0.00	-
3	ACY	C	304	-	1,3,3	1.55	0	0,3,3	0.00	-
2	MPD	S	303	-	7,7,7	0.34	0	9,10,10	0.45	0
2	MPD	G	302	-	7,7,7	0.29	0	9,10,10	0.26	0
2	MPD	X	304	-	7,7,7	0.32	0	9,10,10	0.54	0
3	ACY	W	304	-	1,3,3	1.71	0	0,3,3	0.00	-
2	MPD	B	303	-	7,7,7	0.32	0	9,10,10	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACY	Q	304	-	1,3,3	1.30	0	0,3,3	0.00	-
2	MPD	B	302	-	7,7,7	0.26	0	9,10,10	0.39	0
2	MPD	X	303	-	7,7,7	0.29	0	9,10,10	0.28	0
3	ACY	Z	303	-	1,3,3	1.65	0	0,3,3	0.00	-
3	ACY	O	305	-	1,3,3	1.54	0	0,3,3	0.00	-
2	MPD	T	303	-	7,7,7	0.30	0	9,10,10	0.86	0
3	ACY	D	304	-	1,3,3	1.49	0	0,3,3	0.00	-
2	MPD	W	302	-	7,7,7	0.29	0	9,10,10	0.36	0
3	ACY	J	304	-	1,3,3	1.49	0	0,3,3	0.00	-
2	MPD	P	303	-	7,7,7	0.30	0	9,10,10	0.49	0
2	MPD	J	303	-	7,7,7	0.29	0	9,10,10	0.67	0
3	ACY	b	304	-	1,3,3	1.42	0	0,3,3	0.00	-
2	MPD	L	303	-	7,7,7	0.28	0	9,10,10	0.61	0
2	MPD	R	302	-	7,7,7	0.28	0	9,10,10	0.63	0
2	MPD	O	302	-	7,7,7	0.23	0	9,10,10	0.27	0
2	MPD	Q	302	-	7,7,7	0.23	0	9,10,10	0.61	0
2	MPD	N	302	-	7,7,7	0.25	0	9,10,10	0.44	0
2	MPD	K	302	-	7,7,7	0.25	0	9,10,10	0.37	0
2	MPD	J	302	-	7,7,7	0.39	0	9,10,10	0.73	0
2	MPD	D	302	-	7,7,7	0.35	0	9,10,10	0.72	0
2	MPD	O	303	-	7,7,7	0.33	0	9,10,10	0.56	0
3	ACY	D	305	-	1,3,3	1.55	0	0,3,3	0.00	-
2	MPD	E	302	-	7,7,7	0.29	0	9,10,10	0.26	0
2	MPD	b	302	-	7,7,7	0.27	0	9,10,10	0.46	0
2	MPD	V	303	-	7,7,7	0.30	0	9,10,10	0.69	0
3	ACY	L	304	-	1,3,3	1.34	0	0,3,3	0.00	-
2	MPD	G	303	-	7,7,7	0.34	0	9,10,10	0.51	0
2	MPD	R	303	-	7,7,7	0.28	0	9,10,10	0.52	0
2	MPD	X	302	-	7,7,7	0.28	0	9,10,10	0.54	0
2	MPD	D	303	-	7,7,7	0.30	0	9,10,10	0.24	0
2	MPD	C	303	-	7,7,7	0.32	0	9,10,10	0.51	0
2	MPD	N	303	-	7,7,7	0.34	0	9,10,10	0.58	0
3	ACY	S	305	-	1,3,3	1.48	0	0,3,3	0.00	-
2	MPD	V	302	-	7,7,7	0.26	0	9,10,10	0.36	0
2	MPD	Y	303	-	7,7,7	0.35	0	9,10,10	0.61	0
2	MPD	L	302	-	7,7,7	0.29	0	9,10,10	0.53	0
2	MPD	C	302	-	7,7,7	0.28	0	9,10,10	0.37	0
3	ACY	a	304	-	1,3,3	1.65	0	0,3,3	0.00	-
3	ACY	Y	304	-	1,3,3	1.24	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	H	303	-	-	3/5/5/5	-
2	MPD	Q	303	-	-	1/5/5/5	-
2	MPD	M	302	-	-	0/5/5/5	-
2	MPD	I	302	-	-	2/5/5/5	-
2	MPD	K	303	-	-	1/5/5/5	-
2	MPD	E	303	-	-	1/5/5/5	-
2	MPD	A	302	-	-	5/5/5/5	-
2	MPD	Y	302	-	-	2/5/5/5	-
2	MPD	F	303	-	-	3/5/5/5	-
2	MPD	U	303	-	-	3/5/5/5	-
2	MPD	B	303	-	-	2/5/5/5	-
2	MPD	H	302	-	-	0/5/5/5	-
2	MPD	M	303	-	-	1/5/5/5	-
2	MPD	F	302	-	-	0/5/5/5	-
2	MPD	I	303	-	-	2/5/5/5	-
2	MPD	a	302	-	-	2/5/5/5	-
2	MPD	A	303	-	-	1/5/5/5	-
2	MPD	Z	302	-	-	1/5/5/5	-
2	MPD	T	302	-	-	2/5/5/5	-
2	MPD	S	302	-	-	3/5/5/5	-
2	MPD	P	302	-	-	2/5/5/5	-
2	MPD	U	302	-	-	0/5/5/5	-
2	MPD	L	302	-	-	3/5/5/5	-
2	MPD	W	303	-	-	2/5/5/5	-
2	MPD	b	303	-	-	1/5/5/5	-
2	MPD	D	303	-	-	1/5/5/5	-
2	MPD	S	303	-	-	1/5/5/5	-
2	MPD	G	302	-	-	2/5/5/5	-
2	MPD	X	304	-	-	1/5/5/5	-
2	MPD	B	302	-	-	2/5/5/5	-
2	MPD	X	303	-	-	0/5/5/5	-
2	MPD	a	303	-	-	4/5/5/5	-
2	MPD	T	303	-	-	5/5/5/5	-
2	MPD	W	302	-	-	0/5/5/5	-
2	MPD	P	303	-	-	3/5/5/5	-
2	MPD	J	303	-	-	1/5/5/5	-
2	MPD	L	303	-	-	4/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	R	302	-	-	3/5/5/5	-
2	MPD	O	302	-	-	2/5/5/5	-
2	MPD	Q	302	-	-	2/5/5/5	-
2	MPD	N	302	-	-	2/5/5/5	-
2	MPD	K	302	-	-	1/5/5/5	-
2	MPD	J	302	-	-	2/5/5/5	-
2	MPD	D	302	-	-	2/5/5/5	-
2	MPD	O	303	-	-	2/5/5/5	-
2	MPD	C	302	-	-	1/5/5/5	-
2	MPD	E	302	-	-	2/5/5/5	-
2	MPD	b	302	-	-	1/5/5/5	-
2	MPD	V	303	-	-	4/5/5/5	-
2	MPD	G	303	-	-	2/5/5/5	-
2	MPD	R	303	-	-	1/5/5/5	-
2	MPD	X	302	-	-	2/5/5/5	-
2	MPD	C	303	-	-	3/5/5/5	-
2	MPD	N	303	-	-	2/5/5/5	-
2	MPD	V	302	-	-	2/5/5/5	-
2	MPD	Y	303	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	303	MPD	C2-C3-C4-O4
2	I	302	MPD	C2-C3-C4-O4
2	K	303	MPD	C2-C3-C4-C5
2	E	303	MPD	C2-C3-C4-O4
2	A	302	MPD	O2-C2-C3-C4

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, 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	295/302 (97%)	-0.01	8 (2%) 54 62	27, 45, 75, 108	0
1	B	295/302 (97%)	0.12	12 (4%) 37 44	27, 48, 82, 119	0
1	C	294/302 (97%)	0.16	15 (5%) 28 35	31, 50, 82, 108	0
1	D	295/302 (97%)	0.14	14 (4%) 31 38	33, 53, 83, 118	0
1	E	295/302 (97%)	0.38	30 (10%) 6 9	33, 54, 109, 151	0
1	F	294/302 (97%)	0.29	23 (7%) 13 17	30, 52, 95, 147	0
1	G	294/302 (97%)	0.07	17 (5%) 23 29	27, 50, 89, 127	0
1	H	294/302 (97%)	-0.01	9 (3%) 49 56	29, 46, 71, 100	0
1	I	294/302 (97%)	0.11	9 (3%) 49 56	27, 47, 75, 106	0
1	J	294/302 (97%)	0.07	12 (4%) 37 44	24, 46, 80, 122	0
1	K	295/302 (97%)	0.03	9 (3%) 49 56	27, 45, 76, 111	0
1	L	294/302 (97%)	0.10	13 (4%) 34 41	30, 47, 75, 131	0
1	M	295/302 (97%)	0.28	25 (8%) 10 14	29, 52, 92, 149	0
1	N	294/302 (97%)	0.11	13 (4%) 34 41	28, 51, 87, 117	0
1	O	295/302 (97%)	0.09	19 (6%) 19 25	30, 48, 78, 117	0
1	P	294/302 (97%)	0.11	13 (4%) 34 41	29, 48, 75, 131	0
1	Q	294/302 (97%)	0.22	22 (7%) 14 19	30, 51, 95, 140	0
1	R	294/302 (97%)	0.17	15 (5%) 28 35	32, 49, 77, 99	0
1	S	295/302 (97%)	0.21	17 (5%) 23 29	30, 52, 92, 118	0
1	T	294/302 (97%)	0.06	11 (3%) 41 48	30, 47, 76, 106	0
1	U	295/302 (97%)	0.14	12 (4%) 37 44	28, 49, 85, 128	0
1	V	295/302 (97%)	0.05	12 (4%) 37 44	29, 50, 81, 123	0
1	W	294/302 (97%)	0.21	18 (6%) 21 27	33, 53, 94, 155	0
1	X	294/302 (97%)	0.18	17 (5%) 23 29	33, 53, 96, 127	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	294/302 (97%)	0.22	21 (7%) 16 21	29, 52, 102, 136	0
1	Z	294/302 (97%)	0.16	11 (3%) 41 48	28, 51, 87, 124	0
1	a	294/302 (97%)	0.01	12 (4%) 37 44	28, 45, 74, 123	0
1	b	295/302 (97%)	0.08	13 (4%) 34 41	28, 48, 84, 151	0
All	All	8243/8456 (97%)	0.13	422 (5%) 28 35	24, 49, 86, 155	0

The worst 5 of 422 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	71	GLU	7.9
1	M	295	GLU	7.8
1	E	295	GLU	6.6
1	X	258	LEU	6.6
1	E	258	LEU	5.7

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
2	MPD	Z	302	8/8	0.62	0.40	56,82,97,102	0
2	MPD	J	303	8/8	0.63	0.32	59,79,92,96	0
2	MPD	E	303	8/8	0.66	0.36	61,80,89,100	0
3	ACY	A	305	4/4	0.68	0.33	52,72,90,99	0
2	MPD	Q	303	8/8	0.69	0.43	60,78,87,88	0
2	MPD	U	302	8/8	0.69	0.39	66,82,90,90	0
2	MPD	F	303	8/8	0.69	0.38	68,77,84,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MPD	X	304	8/8	0.70	0.45	68,86,88,93	0
3	ACY	V	304	4/4	0.74	0.33	60,72,75,91	0
3	ACY	S	304	4/4	0.75	0.45	51,79,87,101	0
3	ACY	O	305	4/4	0.75	0.29	65,78,84,87	0
3	ACY	H	305	4/4	0.75	0.27	65,73,81,83	0
2	MPD	M	303	8/8	0.76	0.36	69,75,81,97	0
2	MPD	P	303	8/8	0.76	0.21	59,79,86,88	0
3	ACY	W	304	4/4	0.76	0.18	49,65,70,83	0
3	ACY	a	304	4/4	0.76	0.27	67,68,82,87	0
2	MPD	R	302	8/8	0.77	0.28	60,73,83,86	0
2	MPD	U	303	8/8	0.77	0.29	52,76,87,93	0
2	MPD	J	302	8/8	0.78	0.27	63,72,87,93	0
2	MPD	Q	302	8/8	0.79	0.37	69,76,88,103	0
3	ACY	J	304	4/4	0.79	0.18	61,65,78,90	0
2	MPD	W	302	8/8	0.79	0.22	68,75,83,84	0
2	MPD	X	303	8/8	0.80	0.29	60,74,85,90	0
2	MPD	X	302	8/8	0.81	0.27	70,85,88,89	0
2	MPD	L	303	8/8	0.81	0.26	67,72,98,100	0
2	MPD	B	303	8/8	0.82	0.42	78,85,100,101	0
3	ACY	D	304	4/4	0.82	0.33	58,71,73,80	0
3	ACY	S	305	4/4	0.82	0.24	70,73,79,80	0
2	MPD	H	303	8/8	0.82	0.20	62,70,86,88	0
2	MPD	G	303	8/8	0.84	0.20	59,75,86,97	0
3	ACY	T	304	4/4	0.84	0.22	57,65,76,81	0
2	MPD	C	303	8/8	0.84	0.18	65,76,87,88	0
2	MPD	I	303	8/8	0.84	0.25	61,80,92,99	0
2	MPD	Y	303	8/8	0.84	0.31	64,82,87,93	0
2	MPD	V	303	8/8	0.84	0.29	65,82,90,91	0
2	MPD	G	302	8/8	0.85	0.32	66,72,80,81	0
2	MPD	S	302	8/8	0.85	0.34	68,80,81,85	0
2	MPD	N	303	8/8	0.85	0.18	66,79,90,95	0
2	MPD	D	303	8/8	0.85	0.19	51,71,79,80	0
2	MPD	O	302	8/8	0.85	0.31	68,74,80,82	0
2	MPD	R	303	8/8	0.85	0.26	64,77,82,87	0
2	MPD	a	303	8/8	0.86	0.24	55,80,89,93	0
2	MPD	S	303	8/8	0.86	0.25	64,74,81,94	0
2	MPD	E	302	8/8	0.86	0.16	72,81,85,87	0
2	MPD	W	303	8/8	0.86	0.18	60,80,89,91	0
2	MPD	K	302	8/8	0.87	0.24	66,73,83,90	0
3	ACY	L	304	4/4	0.87	0.27	62,70,82,90	0
2	MPD	K	303	8/8	0.87	0.18	63,78,80,88	0
3	ACY	Z	303	4/4	0.87	0.18	56,71,71,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MPD	O	303	8/8	0.87	0.28	58,75,89,93	0
2	MPD	B	302	8/8	0.87	0.29	65,71,79,82	0
2	MPD	F	302	8/8	0.88	0.31	71,79,91,103	0
2	MPD	I	302	8/8	0.88	0.30	64,68,73,82	0
3	ACY	O	304	4/4	0.88	0.24	59,68,77,86	0
2	MPD	A	303	8/8	0.88	0.18	59,72,85,90	0
2	MPD	N	302	8/8	0.88	0.28	64,77,82,92	0
2	MPD	b	303	8/8	0.89	0.26	64,82,86,87	0
3	ACY	X	305	4/4	0.89	0.42	58,74,85,90	0
2	MPD	M	302	8/8	0.89	0.28	64,73,79,82	0
2	MPD	A	302	8/8	0.89	0.24	58,69,77,81	0
3	ACY	E	304	4/4	0.89	0.42	56,70,75,77	0
2	MPD	Y	302	8/8	0.89	0.29	58,76,88,90	0
2	MPD	T	302	8/8	0.90	0.28	64,68,76,78	0
2	MPD	D	302	8/8	0.90	0.17	65,73,83,85	0
3	ACY	C	304	4/4	0.90	0.19	63,66,74,78	0
2	MPD	b	302	8/8	0.91	0.26	71,74,83,88	0
2	MPD	P	302	8/8	0.91	0.19	54,76,79,80	0
3	ACY	b	304	4/4	0.91	0.17	66,69,91,92	0
2	MPD	a	302	8/8	0.91	0.23	60,74,83,89	0
2	MPD	L	302	8/8	0.91	0.17	59,65,80,89	0
2	MPD	T	303	8/8	0.91	0.23	56,72,85,89	0
3	ACY	M	304	4/4	0.92	0.20	53,58,79,84	0
2	MPD	C	302	8/8	0.92	0.24	67,73,79,82	0
3	ACY	A	304	4/4	0.92	0.09	54,61,73,74	0
3	ACY	Q	304	4/4	0.93	0.28	60,64,80,87	0
2	MPD	V	302	8/8	0.93	0.20	49,61,75,80	0
3	ACY	P	304	4/4	0.93	0.17	63,63,82,97	0
2	MPD	H	302	8/8	0.93	0.24	58,64,75,78	0
3	ACY	D	305	4/4	0.93	0.12	70,71,78,78	0
3	ACY	F	304	4/4	0.93	0.18	69,76,84,85	0
3	ACY	K	304	4/4	0.94	0.21	52,67,72,73	0
3	ACY	K	305	4/4	0.94	0.12	45,68,72,82	0
3	ACY	H	304	4/4	0.95	0.08	53,60,76,79	0
3	ACY	Y	304	4/4	0.96	0.30	64,75,79,82	0

6.5 Other polymers

There are no such residues in this entry.