



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:15 PM UTC

PDB ID : 8OF6 / pdb\_00008of6  
Title : Structure of YtoQ  
Authors : Garbers, T.B.; Neumann, P.; Ficner, R.  
Deposited on : 2023-03-14  
Resolution : 2.10 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

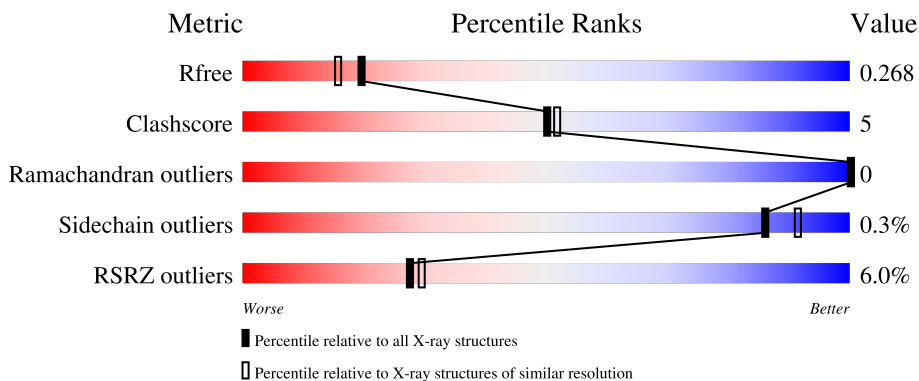
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



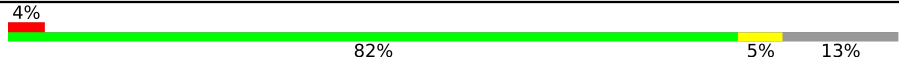
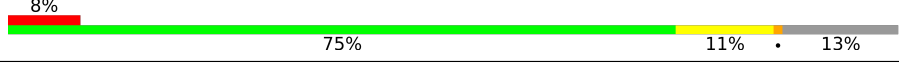



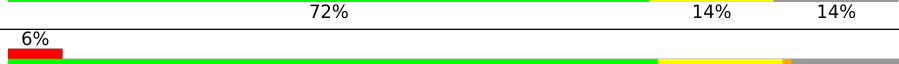
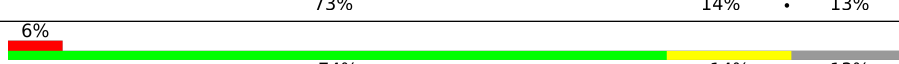
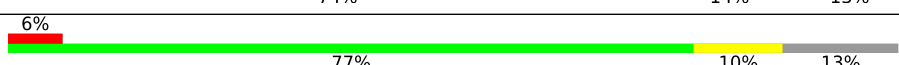
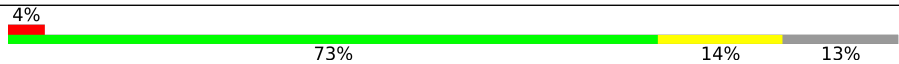


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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	170	 5% 78% 8% 13%
1	B	170	 4% 79% 8% 13%
1	C	170	 6% 75% 12% 13%
1	D	170	 5% 79% 8% 13%
1	E	170	 5% 75% 12% 13%

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Mol	Chain	Length	Quality of chain
1	F	170	 <p>4% 82% 5% 13%</p>
1	G	170	 <p>8% 75% 11% 13%</p>
1	H	170	 <p>3% 77% 10% 13%</p>
1	I	170	 <p>4% 77% 9% 14%</p>
1	J	170	 <p>7% 83% 10% 13%</p>
1	K	170	 <p>6% 72% 14% 14%</p>
1	L	170	 <p>6% 73% 14% 13%</p>
1	M	170	 <p>6% 74% 14% 13%</p>
1	N	170	 <p>6% 77% 10% 13%</p>
1	O	170	 <p>4% 73% 14% 13%</p>
1	P	170	 <p>4% 73% 14% 13%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 38576 atoms, of which 18870 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 YtoQ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	148	2357	753	1179	197	223	5	0	0	0
1	B	148	2367	755	1186	198	223	5	0	0	0
1	C	148	2367	755	1186	198	223	5	0	0	0
1	D	148	2354	752	1177	197	223	5	0	0	0
1	E	148	2352	752	1175	197	223	5	0	0	0
1	F	148	2359	753	1182	198	221	5	0	0	0
1	G	148	2367	755	1186	198	223	5	0	0	0
1	H	148	2357	753	1179	197	223	5	0	0	0
1	I	147	2328	746	1161	195	222	4	0	0	0
1	J	148	2383	761	1192	201	224	5	0	1	0
1	K	147	2334	748	1164	196	222	4	0	0	0
1	L	148	2339	750	1166	197	221	5	0	0	0
1	M	148	2370	758	1183	200	224	5	0	1	0
1	N	148	2383	761	1192	201	224	5	0	1	0
1	O	148	2359	752	1183	196	223	5	0	0	0
1	P	148	2357	752	1179	198	223	5	0	0	0

There are 352 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O34305
A	2	ALA	-	expression tag	UNP O34305
A	3	SER	-	expression tag	UNP O34305
A	4	TRP	-	expression tag	UNP O34305
A	5	SER	-	expression tag	UNP O34305
A	6	HIS	-	expression tag	UNP O34305
A	7	PRO	-	expression tag	UNP O34305
A	8	GLN	-	expression tag	UNP O34305
A	9	PHE	-	expression tag	UNP O34305
A	10	GLU	-	expression tag	UNP O34305
A	11	LYS	-	expression tag	UNP O34305
A	12	GLY	-	expression tag	UNP O34305
A	13	ALA	-	expression tag	UNP O34305
A	14	GLU	-	expression tag	UNP O34305
A	15	THR	-	expression tag	UNP O34305
A	16	ALA	-	expression tag	UNP O34305
A	17	VAL	-	expression tag	UNP O34305
A	18	PRO	-	expression tag	UNP O34305
A	19	ASN	-	expression tag	UNP O34305
A	20	SER	-	expression tag	UNP O34305
A	21	SER	-	expression tag	UNP O34305
A	22	SER	-	expression tag	UNP O34305
B	1	MET	-	initiating methionine	UNP O34305
B	2	ALA	-	expression tag	UNP O34305
B	3	SER	-	expression tag	UNP O34305
B	4	TRP	-	expression tag	UNP O34305
B	5	SER	-	expression tag	UNP O34305
B	6	HIS	-	expression tag	UNP O34305
B	7	PRO	-	expression tag	UNP O34305
B	8	GLN	-	expression tag	UNP O34305
B	9	PHE	-	expression tag	UNP O34305
B	10	GLU	-	expression tag	UNP O34305
B	11	LYS	-	expression tag	UNP O34305
B	12	GLY	-	expression tag	UNP O34305
B	13	ALA	-	expression tag	UNP O34305
B	14	GLU	-	expression tag	UNP O34305
B	15	THR	-	expression tag	UNP O34305
B	16	ALA	-	expression tag	UNP O34305
B	17	VAL	-	expression tag	UNP O34305
B	18	PRO	-	expression tag	UNP O34305
B	19	ASN	-	expression tag	UNP O34305
B	20	SER	-	expression tag	UNP O34305

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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	SER	-	expression tag	UNP O34305
B	22	SER	-	expression tag	UNP O34305
C	1	MET	-	initiating methionine	UNP O34305
C	2	ALA	-	expression tag	UNP O34305
C	3	SER	-	expression tag	UNP O34305
C	4	TRP	-	expression tag	UNP O34305
C	5	SER	-	expression tag	UNP O34305
C	6	HIS	-	expression tag	UNP O34305
C	7	PRO	-	expression tag	UNP O34305
C	8	GLN	-	expression tag	UNP O34305
C	9	PHE	-	expression tag	UNP O34305
C	10	GLU	-	expression tag	UNP O34305
C	11	LYS	-	expression tag	UNP O34305
C	12	GLY	-	expression tag	UNP O34305
C	13	ALA	-	expression tag	UNP O34305
C	14	GLU	-	expression tag	UNP O34305
C	15	THR	-	expression tag	UNP O34305
C	16	ALA	-	expression tag	UNP O34305
C	17	VAL	-	expression tag	UNP O34305
C	18	PRO	-	expression tag	UNP O34305
C	19	ASN	-	expression tag	UNP O34305
C	20	SER	-	expression tag	UNP O34305
C	21	SER	-	expression tag	UNP O34305
C	22	SER	-	expression tag	UNP O34305
D	1	MET	-	initiating methionine	UNP O34305
D	2	ALA	-	expression tag	UNP O34305
D	3	SER	-	expression tag	UNP O34305
D	4	TRP	-	expression tag	UNP O34305
D	5	SER	-	expression tag	UNP O34305
D	6	HIS	-	expression tag	UNP O34305
D	7	PRO	-	expression tag	UNP O34305
D	8	GLN	-	expression tag	UNP O34305
D	9	PHE	-	expression tag	UNP O34305
D	10	GLU	-	expression tag	UNP O34305
D	11	LYS	-	expression tag	UNP O34305
D	12	GLY	-	expression tag	UNP O34305
D	13	ALA	-	expression tag	UNP O34305
D	14	GLU	-	expression tag	UNP O34305
D	15	THR	-	expression tag	UNP O34305
D	16	ALA	-	expression tag	UNP O34305
D	17	VAL	-	expression tag	UNP O34305
D	18	PRO	-	expression tag	UNP O34305

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	ASN	-	expression tag	UNP O34305
D	20	SER	-	expression tag	UNP O34305
D	21	SER	-	expression tag	UNP O34305
D	22	SER	-	expression tag	UNP O34305
E	1	MET	-	initiating methionine	UNP O34305
E	2	ALA	-	expression tag	UNP O34305
E	3	SER	-	expression tag	UNP O34305
E	4	TRP	-	expression tag	UNP O34305
E	5	SER	-	expression tag	UNP O34305
E	6	HIS	-	expression tag	UNP O34305
E	7	PRO	-	expression tag	UNP O34305
E	8	GLN	-	expression tag	UNP O34305
E	9	PHE	-	expression tag	UNP O34305
E	10	GLU	-	expression tag	UNP O34305
E	11	LYS	-	expression tag	UNP O34305
E	12	GLY	-	expression tag	UNP O34305
E	13	ALA	-	expression tag	UNP O34305
E	14	GLU	-	expression tag	UNP O34305
E	15	THR	-	expression tag	UNP O34305
E	16	ALA	-	expression tag	UNP O34305
E	17	VAL	-	expression tag	UNP O34305
E	18	PRO	-	expression tag	UNP O34305
E	19	ASN	-	expression tag	UNP O34305
E	20	SER	-	expression tag	UNP O34305
E	21	SER	-	expression tag	UNP O34305
E	22	SER	-	expression tag	UNP O34305
F	1	MET	-	initiating methionine	UNP O34305
F	2	ALA	-	expression tag	UNP O34305
F	3	SER	-	expression tag	UNP O34305
F	4	TRP	-	expression tag	UNP O34305
F	5	SER	-	expression tag	UNP O34305
F	6	HIS	-	expression tag	UNP O34305
F	7	PRO	-	expression tag	UNP O34305
F	8	GLN	-	expression tag	UNP O34305
F	9	PHE	-	expression tag	UNP O34305
F	10	GLU	-	expression tag	UNP O34305
F	11	LYS	-	expression tag	UNP O34305
F	12	GLY	-	expression tag	UNP O34305
F	13	ALA	-	expression tag	UNP O34305
F	14	GLU	-	expression tag	UNP O34305
F	15	THR	-	expression tag	UNP O34305
F	16	ALA	-	expression tag	UNP O34305

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Chain	Residue	Modelled	Actual	Comment	Reference
F	17	VAL	-	expression tag	UNP O34305
F	18	PRO	-	expression tag	UNP O34305
F	19	ASN	-	expression tag	UNP O34305
F	20	SER	-	expression tag	UNP O34305
F	21	SER	-	expression tag	UNP O34305
F	22	SER	-	expression tag	UNP O34305
G	1	MET	-	initiating methionine	UNP O34305
G	2	ALA	-	expression tag	UNP O34305
G	3	SER	-	expression tag	UNP O34305
G	4	TRP	-	expression tag	UNP O34305
G	5	SER	-	expression tag	UNP O34305
G	6	HIS	-	expression tag	UNP O34305
G	7	PRO	-	expression tag	UNP O34305
G	8	GLN	-	expression tag	UNP O34305
G	9	PHE	-	expression tag	UNP O34305
G	10	GLU	-	expression tag	UNP O34305
G	11	LYS	-	expression tag	UNP O34305
G	12	GLY	-	expression tag	UNP O34305
G	13	ALA	-	expression tag	UNP O34305
G	14	GLU	-	expression tag	UNP O34305
G	15	THR	-	expression tag	UNP O34305
G	16	ALA	-	expression tag	UNP O34305
G	17	VAL	-	expression tag	UNP O34305
G	18	PRO	-	expression tag	UNP O34305
G	19	ASN	-	expression tag	UNP O34305
G	20	SER	-	expression tag	UNP O34305
G	21	SER	-	expression tag	UNP O34305
G	22	SER	-	expression tag	UNP O34305
H	1	MET	-	initiating methionine	UNP O34305
H	2	ALA	-	expression tag	UNP O34305
H	3	SER	-	expression tag	UNP O34305
H	4	TRP	-	expression tag	UNP O34305
H	5	SER	-	expression tag	UNP O34305
H	6	HIS	-	expression tag	UNP O34305
H	7	PRO	-	expression tag	UNP O34305
H	8	GLN	-	expression tag	UNP O34305
H	9	PHE	-	expression tag	UNP O34305
H	10	GLU	-	expression tag	UNP O34305
H	11	LYS	-	expression tag	UNP O34305
H	12	GLY	-	expression tag	UNP O34305
H	13	ALA	-	expression tag	UNP O34305
H	14	GLU	-	expression tag	UNP O34305

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Chain	Residue	Modelled	Actual	Comment	Reference
H	15	THR	-	expression tag	UNP O34305
H	16	ALA	-	expression tag	UNP O34305
H	17	VAL	-	expression tag	UNP O34305
H	18	PRO	-	expression tag	UNP O34305
H	19	ASN	-	expression tag	UNP O34305
H	20	SER	-	expression tag	UNP O34305
H	21	SER	-	expression tag	UNP O34305
H	22	SER	-	expression tag	UNP O34305
I	1	MET	-	initiating methionine	UNP O34305
I	2	ALA	-	expression tag	UNP O34305
I	3	SER	-	expression tag	UNP O34305
I	4	TRP	-	expression tag	UNP O34305
I	5	SER	-	expression tag	UNP O34305
I	6	HIS	-	expression tag	UNP O34305
I	7	PRO	-	expression tag	UNP O34305
I	8	GLN	-	expression tag	UNP O34305
I	9	PHE	-	expression tag	UNP O34305
I	10	GLU	-	expression tag	UNP O34305
I	11	LYS	-	expression tag	UNP O34305
I	12	GLY	-	expression tag	UNP O34305
I	13	ALA	-	expression tag	UNP O34305
I	14	GLU	-	expression tag	UNP O34305
I	15	THR	-	expression tag	UNP O34305
I	16	ALA	-	expression tag	UNP O34305
I	17	VAL	-	expression tag	UNP O34305
I	18	PRO	-	expression tag	UNP O34305
I	19	ASN	-	expression tag	UNP O34305
I	20	SER	-	expression tag	UNP O34305
I	21	SER	-	expression tag	UNP O34305
I	22	SER	-	expression tag	UNP O34305
J	1	MET	-	initiating methionine	UNP O34305
J	2	ALA	-	expression tag	UNP O34305
J	3	SER	-	expression tag	UNP O34305
J	4	TRP	-	expression tag	UNP O34305
J	5	SER	-	expression tag	UNP O34305
J	6	HIS	-	expression tag	UNP O34305
J	7	PRO	-	expression tag	UNP O34305
J	8	GLN	-	expression tag	UNP O34305
J	9	PHE	-	expression tag	UNP O34305
J	10	GLU	-	expression tag	UNP O34305
J	11	LYS	-	expression tag	UNP O34305
J	12	GLY	-	expression tag	UNP O34305

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Chain	Residue	Modelled	Actual	Comment	Reference
J	13	ALA	-	expression tag	UNP O34305
J	14	GLU	-	expression tag	UNP O34305
J	15	THR	-	expression tag	UNP O34305
J	16	ALA	-	expression tag	UNP O34305
J	17	VAL	-	expression tag	UNP O34305
J	18	PRO	-	expression tag	UNP O34305
J	19	ASN	-	expression tag	UNP O34305
J	20	SER	-	expression tag	UNP O34305
J	21	SER	-	expression tag	UNP O34305
J	22	SER	-	expression tag	UNP O34305
K	1	MET	-	initiating methionine	UNP O34305
K	2	ALA	-	expression tag	UNP O34305
K	3	SER	-	expression tag	UNP O34305
K	4	TRP	-	expression tag	UNP O34305
K	5	SER	-	expression tag	UNP O34305
K	6	HIS	-	expression tag	UNP O34305
K	7	PRO	-	expression tag	UNP O34305
K	8	GLN	-	expression tag	UNP O34305
K	9	PHE	-	expression tag	UNP O34305
K	10	GLU	-	expression tag	UNP O34305
K	11	LYS	-	expression tag	UNP O34305
K	12	GLY	-	expression tag	UNP O34305
K	13	ALA	-	expression tag	UNP O34305
K	14	GLU	-	expression tag	UNP O34305
K	15	THR	-	expression tag	UNP O34305
K	16	ALA	-	expression tag	UNP O34305
K	17	VAL	-	expression tag	UNP O34305
K	18	PRO	-	expression tag	UNP O34305
K	19	ASN	-	expression tag	UNP O34305
K	20	SER	-	expression tag	UNP O34305
K	21	SER	-	expression tag	UNP O34305
K	22	SER	-	expression tag	UNP O34305
L	1	MET	-	initiating methionine	UNP O34305
L	2	ALA	-	expression tag	UNP O34305
L	3	SER	-	expression tag	UNP O34305
L	4	TRP	-	expression tag	UNP O34305
L	5	SER	-	expression tag	UNP O34305
L	6	HIS	-	expression tag	UNP O34305
L	7	PRO	-	expression tag	UNP O34305
L	8	GLN	-	expression tag	UNP O34305
L	9	PHE	-	expression tag	UNP O34305
L	10	GLU	-	expression tag	UNP O34305

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Chain	Residue	Modelled	Actual	Comment	Reference
L	11	LYS	-	expression tag	UNP O34305
L	12	GLY	-	expression tag	UNP O34305
L	13	ALA	-	expression tag	UNP O34305
L	14	GLU	-	expression tag	UNP O34305
L	15	THR	-	expression tag	UNP O34305
L	16	ALA	-	expression tag	UNP O34305
L	17	VAL	-	expression tag	UNP O34305
L	18	PRO	-	expression tag	UNP O34305
L	19	ASN	-	expression tag	UNP O34305
L	20	SER	-	expression tag	UNP O34305
L	21	SER	-	expression tag	UNP O34305
L	22	SER	-	expression tag	UNP O34305
M	1	MET	-	initiating methionine	UNP O34305
M	2	ALA	-	expression tag	UNP O34305
M	3	SER	-	expression tag	UNP O34305
M	4	TRP	-	expression tag	UNP O34305
M	5	SER	-	expression tag	UNP O34305
M	6	HIS	-	expression tag	UNP O34305
M	7	PRO	-	expression tag	UNP O34305
M	8	GLN	-	expression tag	UNP O34305
M	9	PHE	-	expression tag	UNP O34305
M	10	GLU	-	expression tag	UNP O34305
M	11	LYS	-	expression tag	UNP O34305
M	12	GLY	-	expression tag	UNP O34305
M	13	ALA	-	expression tag	UNP O34305
M	14	GLU	-	expression tag	UNP O34305
M	15	THR	-	expression tag	UNP O34305
M	16	ALA	-	expression tag	UNP O34305
M	17	VAL	-	expression tag	UNP O34305
M	18	PRO	-	expression tag	UNP O34305
M	19	ASN	-	expression tag	UNP O34305
M	20	SER	-	expression tag	UNP O34305
M	21	SER	-	expression tag	UNP O34305
M	22	SER	-	expression tag	UNP O34305
N	1	MET	-	initiating methionine	UNP O34305
N	2	ALA	-	expression tag	UNP O34305
N	3	SER	-	expression tag	UNP O34305
N	4	TRP	-	expression tag	UNP O34305
N	5	SER	-	expression tag	UNP O34305
N	6	HIS	-	expression tag	UNP O34305
N	7	PRO	-	expression tag	UNP O34305
N	8	GLN	-	expression tag	UNP O34305

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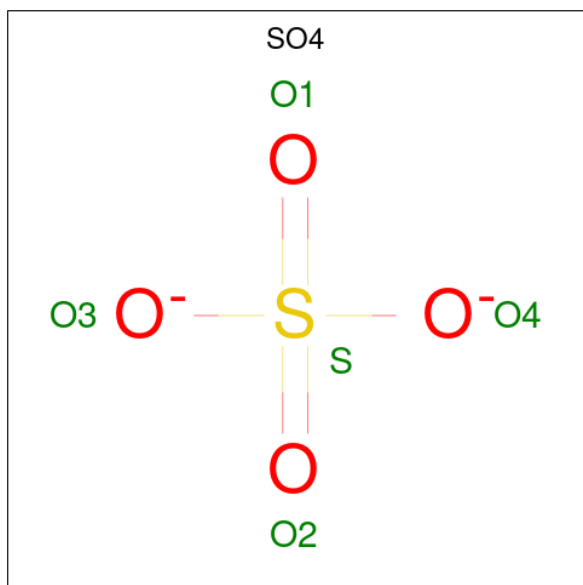
Chain	Residue	Modelled	Actual	Comment	Reference
N	9	PHE	-	expression tag	UNP O34305
N	10	GLU	-	expression tag	UNP O34305
N	11	LYS	-	expression tag	UNP O34305
N	12	GLY	-	expression tag	UNP O34305
N	13	ALA	-	expression tag	UNP O34305
N	14	GLU	-	expression tag	UNP O34305
N	15	THR	-	expression tag	UNP O34305
N	16	ALA	-	expression tag	UNP O34305
N	17	VAL	-	expression tag	UNP O34305
N	18	PRO	-	expression tag	UNP O34305
N	19	ASN	-	expression tag	UNP O34305
N	20	SER	-	expression tag	UNP O34305
N	21	SER	-	expression tag	UNP O34305
N	22	SER	-	expression tag	UNP O34305
O	1	MET	-	initiating methionine	UNP O34305
O	2	ALA	-	expression tag	UNP O34305
O	3	SER	-	expression tag	UNP O34305
O	4	TRP	-	expression tag	UNP O34305
O	5	SER	-	expression tag	UNP O34305
O	6	HIS	-	expression tag	UNP O34305
O	7	PRO	-	expression tag	UNP O34305
O	8	GLN	-	expression tag	UNP O34305
O	9	PHE	-	expression tag	UNP O34305
O	10	GLU	-	expression tag	UNP O34305
O	11	LYS	-	expression tag	UNP O34305
O	12	GLY	-	expression tag	UNP O34305
O	13	ALA	-	expression tag	UNP O34305
O	14	GLU	-	expression tag	UNP O34305
O	15	THR	-	expression tag	UNP O34305
O	16	ALA	-	expression tag	UNP O34305
O	17	VAL	-	expression tag	UNP O34305
O	18	PRO	-	expression tag	UNP O34305
O	19	ASN	-	expression tag	UNP O34305
O	20	SER	-	expression tag	UNP O34305
O	21	SER	-	expression tag	UNP O34305
O	22	SER	-	expression tag	UNP O34305
P	1	MET	-	initiating methionine	UNP O34305
P	2	ALA	-	expression tag	UNP O34305
P	3	SER	-	expression tag	UNP O34305
P	4	TRP	-	expression tag	UNP O34305
P	5	SER	-	expression tag	UNP O34305
P	6	HIS	-	expression tag	UNP O34305

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Chain	Residue	Modelled	Actual	Comment	Reference
P	7	PRO	-	expression tag	UNP O34305
P	8	GLN	-	expression tag	UNP O34305
P	9	PHE	-	expression tag	UNP O34305
P	10	GLU	-	expression tag	UNP O34305
P	11	LYS	-	expression tag	UNP O34305
P	12	GLY	-	expression tag	UNP O34305
P	13	ALA	-	expression tag	UNP O34305
P	14	GLU	-	expression tag	UNP O34305
P	15	THR	-	expression tag	UNP O34305
P	16	ALA	-	expression tag	UNP O34305
P	17	VAL	-	expression tag	UNP O34305
P	18	PRO	-	expression tag	UNP O34305
P	19	ASN	-	expression tag	UNP O34305
P	20	SER	-	expression tag	UNP O34305
P	21	SER	-	expression tag	UNP O34305
P	22	SER	-	expression tag	UNP O34305

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

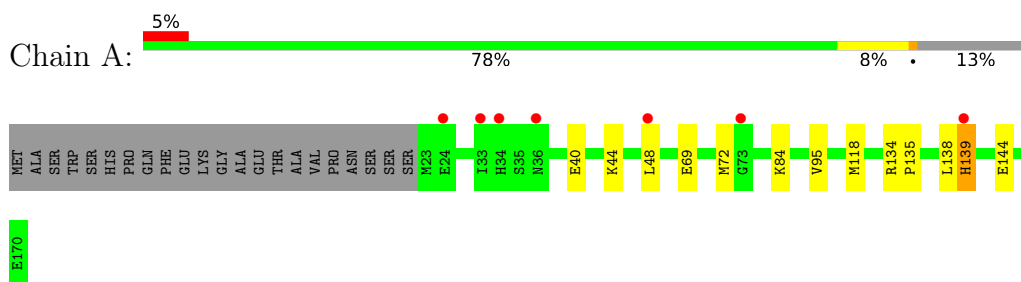
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total 60	O 60	0	0
3	B	70	Total 70	O 70	0	0
3	C	68	Total 68	O 68	0	0
3	D	47	Total 47	O 47	0	0
3	E	68	Total 68	O 68	0	0
3	F	62	Total 62	O 62	0	0
3	G	63	Total 63	O 63	0	0
3	H	72	Total 72	O 72	0	0
3	I	37	Total 37	O 37	0	0
3	J	49	Total 49	O 49	0	0
3	K	46	Total 46	O 46	0	0
3	L	48	Total 48	O 48	0	0
3	M	40	Total 40	O 40	0	0
3	N	38	Total 38	O 38	0	0
3	O	32	Total 32	O 32	0	0
3	P	33	Total 33	O 33	0	0

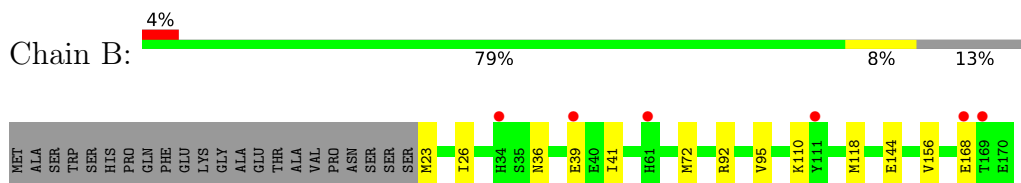
### 3 Residue-property plots [i](#)

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.

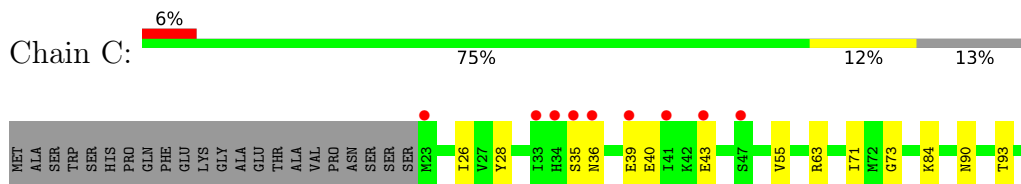
- Molecule 1: YtoQ



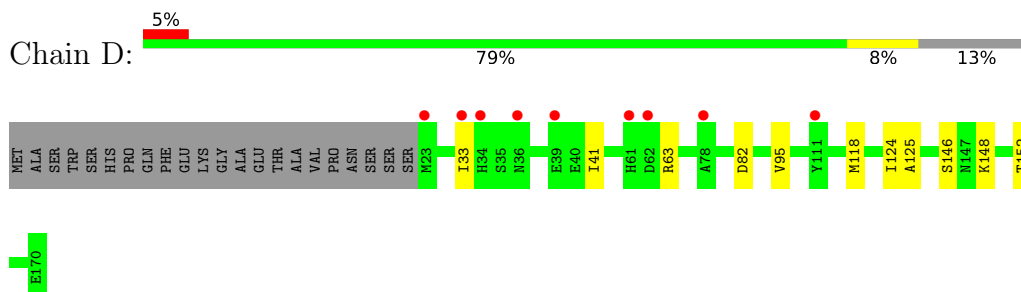
- Molecule 1: YtoQ



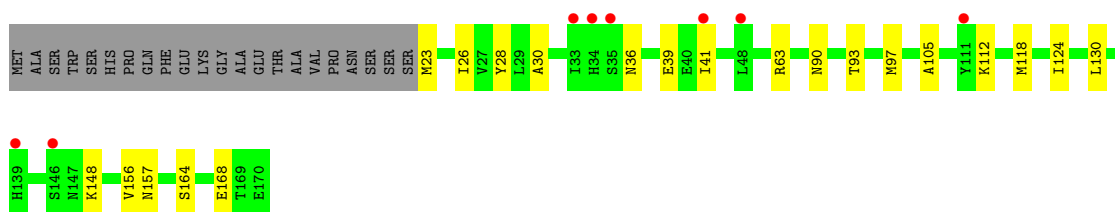
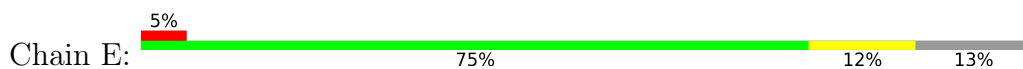
- Molecule 1: YtoQ



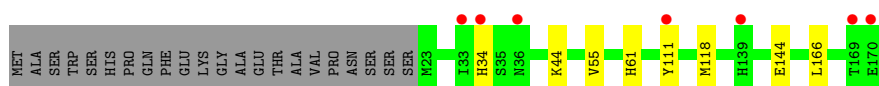
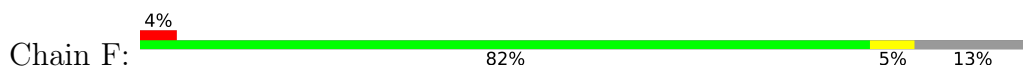
- Molecule 1: YtoQ



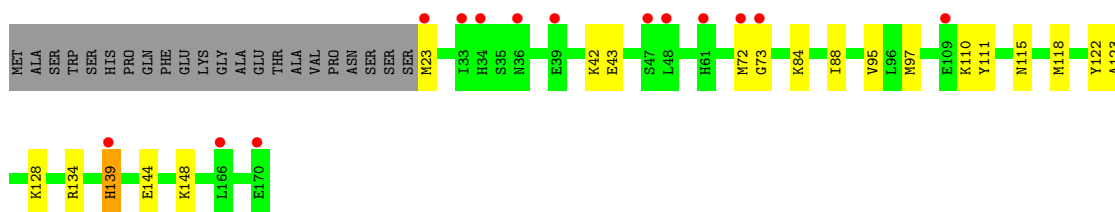
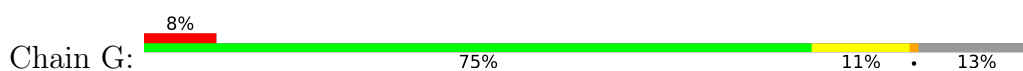
- Molecule 1: YtoQ



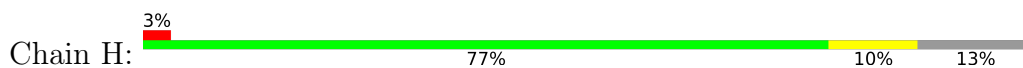
- Molecule 1: YtoQ



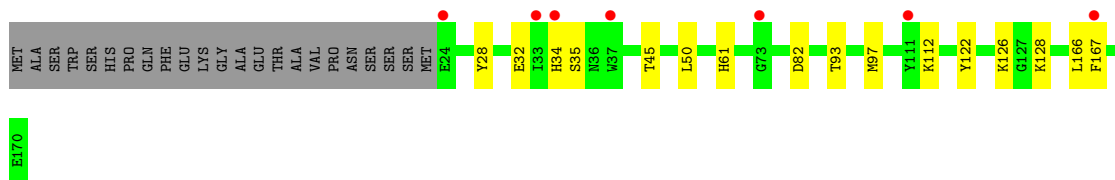
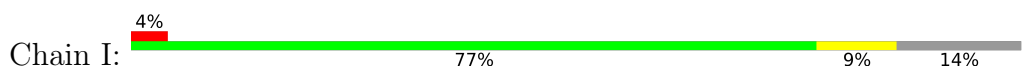
- Molecule 1: YtoQ



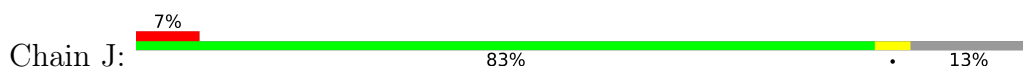
- Molecule 1: YtoQ

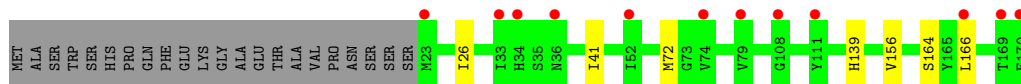


- Molecule 1: YtoQ

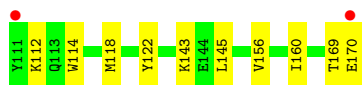


- Molecule 1: YtoQ

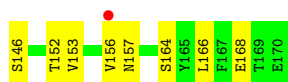
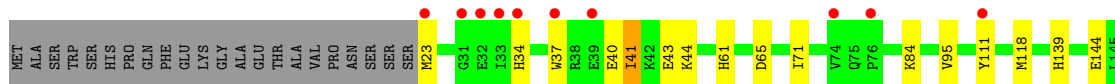




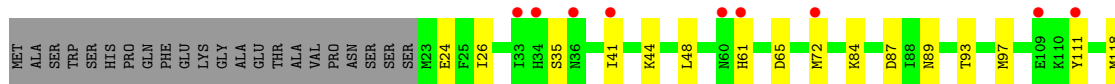
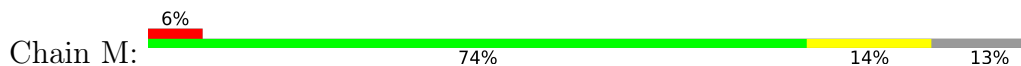
• Molecule 1: YtoQ



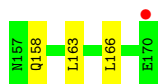
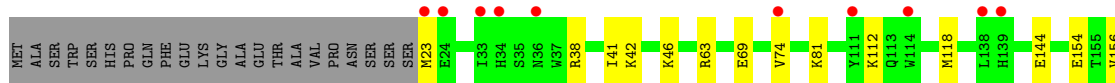
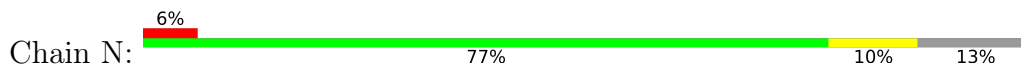
• Molecule 1: YtoQ



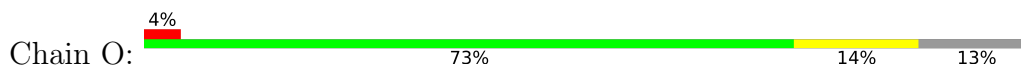
• Molecule 1: YtoQ

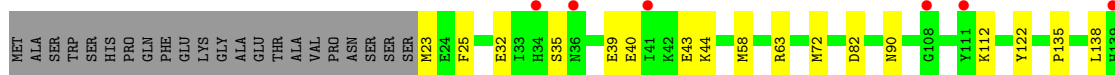


• Molecule 1: YtoQ

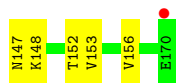
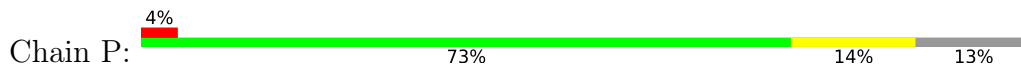


• Molecule 1: YtoQ





• Molecule 1: YtoQ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.34Å 70.15Å 149.94Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	49.45 – 2.10 49.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.45-2.10) 98.8 (49.45-2.10)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.227 , 0.268 0.227 , 0.268	Depositor DCC
$R_{free}$ test set	8098 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	38576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.61 % 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 9.1383e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.43	0/1201	0.61	1/1623 (0.1%)
1	B	0.51	0/1204	0.69	0/1626
1	C	0.55	1/1204 (0.1%)	0.70	2/1626 (0.1%)
1	D	0.56	2/1200 (0.2%)	0.73	1/1622 (0.1%)
1	E	0.59	0/1200	0.85	1/1622 (0.1%)
1	F	0.45	0/1200	0.64	0/1621
1	G	0.55	2/1204 (0.2%)	0.74	2/1626 (0.1%)
1	H	0.58	2/1201 (0.2%)	0.70	0/1623
1	I	0.45	0/1190	0.62	1/1610 (0.1%)
1	J	0.53	0/1215	0.74	0/1641
1	K	0.50	0/1193	0.73	1/1613 (0.1%)
1	L	0.57	1/1196 (0.1%)	0.78	1/1617 (0.1%)
1	M	0.44	0/1211	0.66	2/1637 (0.1%)
1	N	0.53	0/1215	0.81	2/1641 (0.1%)
1	O	0.58	2/1198 (0.2%)	0.77	1/1618 (0.1%)
1	P	0.51	0/1201	0.76	0/1621
All	All	0.52	10/19233 (0.1%)	0.73	15/25987 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	43	GLU	C-O	-7.45	1.15	1.24
1	O	122	TYR	C-O	-6.96	1.16	1.24
1	C	40	GLU	C-O	-6.57	1.16	1.24
1	D	165	TYR	C-O	-5.93	1.17	1.24
1	D	125	ALA	C-O	-5.80	1.17	1.24

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	112	LYS	CA-C-O	-6.87	113.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	HIS	CA-CB-CG	-6.34	107.46	113.80
1	K	55	VAL	CA-C-O	-6.29	115.25	121.67
1	D	33	ILE	N-CA-C	-6.18	106.48	112.29
1	G	43	GLU	CA-C-O	-6.15	114.57	120.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1178	1179	1181	13	0
1	B	1181	1186	1190	16	0
1	C	1181	1186	1190	15	0
1	D	1177	1177	1179	8	0
1	E	1177	1175	1179	16	0
1	F	1177	1182	1186	11	0
1	G	1181	1186	1190	18	0
1	H	1178	1179	1181	14	0
1	I	1167	1161	1163	12	0
1	J	1191	1192	1196	6	0
1	K	1170	1164	1172	25	0
1	L	1173	1166	1175	23	0
1	M	1187	1183	1185	15	0
1	N	1191	1192	1196	11	0
1	O	1176	1183	1185	17	0
1	P	1178	1179	1182	26	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	60	0	0	1	0
3	B	70	0	0	1	0
3	C	68	0	0	3	0
3	D	47	0	0	0	0
3	E	68	0	0	1	0
3	F	62	0	0	1	0
3	G	63	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	72	0	0	3	0
3	I	37	0	0	1	0
3	J	49	0	0	1	0
3	K	46	0	0	4	0
3	L	48	0	0	0	0
3	M	40	0	0	2	0
3	N	38	0	0	0	0
3	O	32	0	0	0	0
3	P	33	0	0	0	0
All	All	19706	18870	18930	199	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 199 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:41:ILE:HD13	1:K:160:ILE:HD11	1.46	0.94
1:I:28:TYR:OH	1:I:93:THR:HG22	1.74	0.86
1:K:41:ILE:CD1	1:K:156:VAL:HG13	2.06	0.85
1:K:41:ILE:HD13	1:K:156:VAL:HG13	1.59	0.84
1:M:24:GLU:OE1	1:M:24:GLU:N	2.13	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	146/170 (86%)	144 (99%)	2 (1%)	0	100 100
1	B	146/170 (86%)	144 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	146/170 (86%)	145 (99%)	1 (1%)	0	100	100
1	D	146/170 (86%)	145 (99%)	1 (1%)	0	100	100
1	E	146/170 (86%)	144 (99%)	2 (1%)	0	100	100
1	F	146/170 (86%)	144 (99%)	2 (1%)	0	100	100
1	G	146/170 (86%)	143 (98%)	3 (2%)	0	100	100
1	H	146/170 (86%)	144 (99%)	2 (1%)	0	100	100
1	I	145/170 (85%)	142 (98%)	3 (2%)	0	100	100
1	J	147/170 (86%)	144 (98%)	3 (2%)	0	100	100
1	K	145/170 (85%)	143 (99%)	2 (1%)	0	100	100
1	L	146/170 (86%)	143 (98%)	3 (2%)	0	100	100
1	M	147/170 (86%)	145 (99%)	2 (1%)	0	100	100
1	N	147/170 (86%)	144 (98%)	3 (2%)	0	100	100
1	O	146/170 (86%)	143 (98%)	3 (2%)	0	100	100
1	P	146/170 (86%)	144 (99%)	2 (1%)	0	100	100
All	All	2337/2720 (86%)	2301 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/147 (87%)	128 (100%)	0	100	100
1	B	129/147 (88%)	129 (100%)	0	100	100
1	C	129/147 (88%)	128 (99%)	1 (1%)	73	81
1	D	128/147 (87%)	128 (100%)	0	100	100
1	E	128/147 (87%)	128 (100%)	0	100	100
1	F	128/147 (87%)	128 (100%)	0	100	100
1	G	129/147 (88%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	128/147 (87%)	128 (100%)	0	100	100
1	I	126/147 (86%)	126 (100%)	0	100	100
1	J	130/147 (88%)	129 (99%)	1 (1%)	73	81
1	K	127/147 (86%)	127 (100%)	0	100	100
1	L	127/147 (86%)	127 (100%)	0	100	100
1	M	129/147 (88%)	127 (98%)	2 (2%)	55	64
1	N	130/147 (88%)	130 (100%)	0	100	100
1	O	128/147 (87%)	126 (98%)	2 (2%)	55	64
1	P	128/147 (87%)	128 (100%)	0	100	100
All	All	2052/2352 (87%)	2046 (100%)	6 (0%)	86	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	155	THR
1	O	32	GLU
1	O	35	SER
1	J	164	SER
1	C	35	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	36	ASN
1	L	75	GLN
1	K	139	HIS
1	M	34	HIS
1	C	140	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	C	201	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	B	201	-	4,4,4	0.41	0	6,6,6	0.12	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	148/170 (87%)	0.46	8 (5%) 31 33	29, 41, 62, 71	0
1	B	148/170 (87%)	0.27	6 (4%) 41 43	27, 38, 56, 64	1 (0%)
1	C	148/170 (87%)	0.36	11 (7%) 20 22	27, 40, 59, 71	0
1	D	148/170 (87%)	0.44	9 (6%) 27 29	28, 40, 60, 76	0
1	E	148/170 (87%)	0.50	8 (5%) 31 33	29, 41, 60, 71	0
1	F	148/170 (87%)	0.41	7 (4%) 36 38	27, 39, 56, 73	0
1	G	148/170 (87%)	0.58	14 (9%) 14 14	29, 40, 63, 71	0
1	H	148/170 (87%)	0.23	5 (3%) 48 50	27, 38, 54, 64	0
1	I	147/170 (86%)	0.46	7 (4%) 35 38	30, 47, 66, 77	0
1	J	148/170 (87%)	0.69	12 (8%) 18 19	22, 46, 66, 81	1 (0%)
1	K	147/170 (86%)	0.58	11 (7%) 20 21	34, 49, 68, 81	0
1	L	148/170 (87%)	0.66	11 (7%) 20 22	30, 47, 65, 74	2 (1%)
1	M	148/170 (87%)	0.60	11 (7%) 20 22	25, 45, 67, 75	1 (0%)
1	N	148/170 (87%)	0.50	11 (7%) 20 22	22, 45, 63, 70	2 (1%)
1	O	148/170 (87%)	0.63	6 (4%) 41 43	32, 48, 66, 77	0
1	P	148/170 (87%)	0.57	6 (4%) 41 43	30, 47, 66, 76	2 (1%)
All	All	2366/2720 (86%)	0.50	143 (6%) 27 29	22, 43, 64, 81	9 (0%)

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	74	VAL	5.2
1	A	33	ILE	5.0
1	D	111	TYR	4.8
1	N	139[A]	HIS	4.6
1	A	34	HIS	4.3

## 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 oligosaccharides 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, 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	C	201	5/5	0.53	0.10	75,86,92,108	0
2	SO4	B	201	5/5	0.84	0.12	47,59,63,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.