Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2024 – 12:29 pm GMT

PDB ID	:	8OF6
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

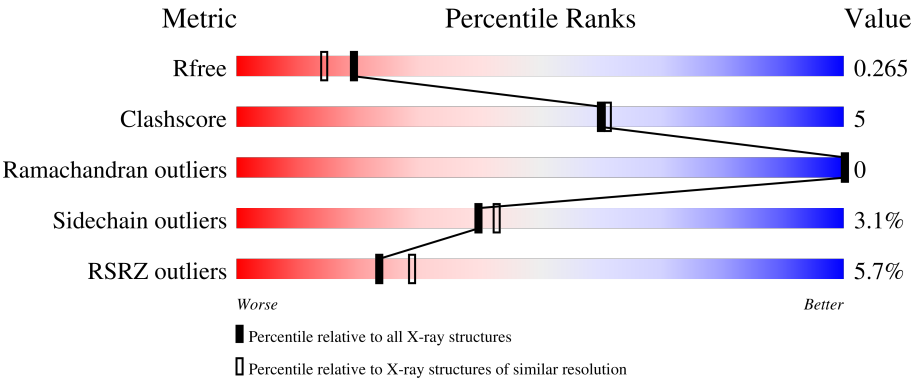
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	170	6% 79% 6% • 13%
1	B	170	3% 79% 7% • 13%
1	C	170	6% 75% 11% • 13%
1	D	170	5% 79% 8% 13%
1	E	170	3% 74% 13% 13%

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Mol	Chain	Length	Quality of chain
1	F	170	3% 83% 13%
1	G	170	6% 78% 9% 13%
1	H	170	4% 78% 9% 13%
1	I	170	6% 76% 10% 14%
1	J	170	6% 81% 6% 13%
1	K	170	9% 73% 13% 14%
1	L	170	4% 73% 14% 13%
1	M	170	4% 74% 13% 13%
1	N	170	5% 78% 9% 13%
1	O	170	5% 73% 14% 13%
1	P	170	4% 69% 18% 13%

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

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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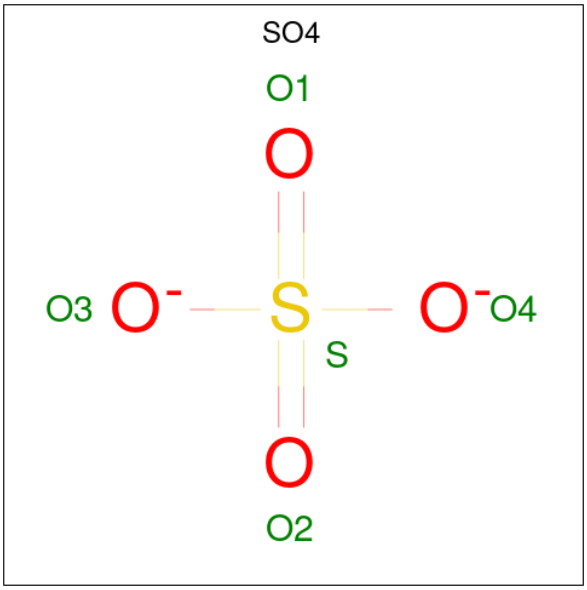
Chain	Residue	Modelled	Actual	Comment	Reference
P	7	PRO	-	expression tag	UNP O34305
P	8	GLN	-	expression tag	UNP O34305
P	9	PHE	-	expression tag	UNP O34305
P	10	GLU	-	expression tag	UNP O34305
P	11	LYS	-	expression tag	UNP O34305
P	12	GLY	-	expression tag	UNP O34305
P	13	ALA	-	expression tag	UNP O34305
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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

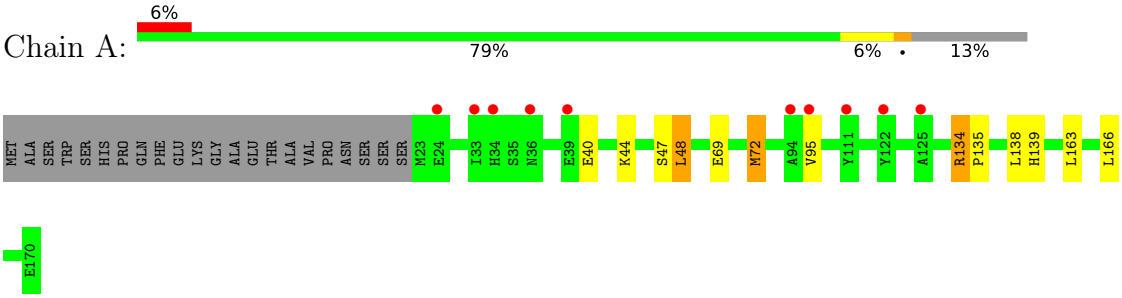
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	60	Total O 60 60	0	0
3	B	70	Total O 70 70	0	0
3	C	68	Total O 68 68	0	0
3	D	47	Total O 47 47	0	0
3	E	68	Total O 68 68	0	0
3	F	62	Total O 62 62	0	0
3	G	63	Total O 63 63	0	0
3	H	72	Total O 72 72	0	0
3	I	37	Total O 37 37	0	0
3	J	49	Total O 49 49	0	0
3	K	46	Total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

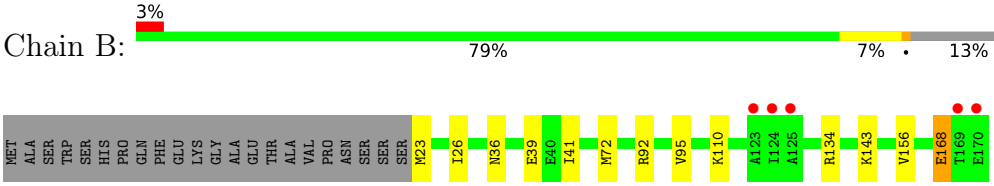
• Molecule 1: YtoQ

Chain A:



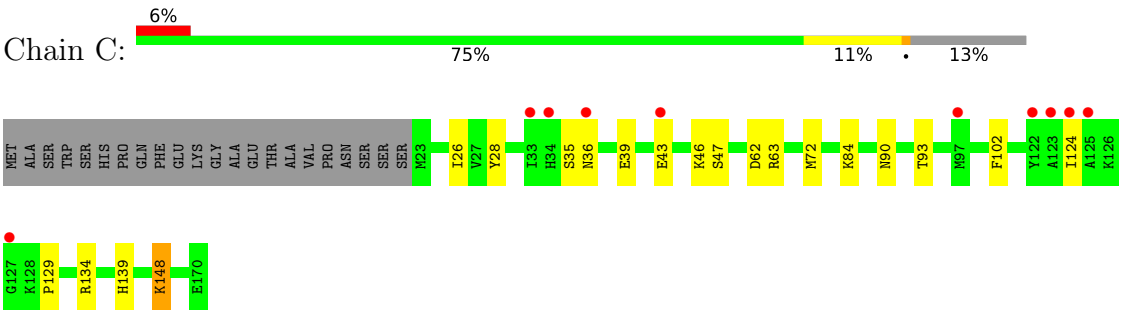
• Molecule 1: YtoQ

Chain B:



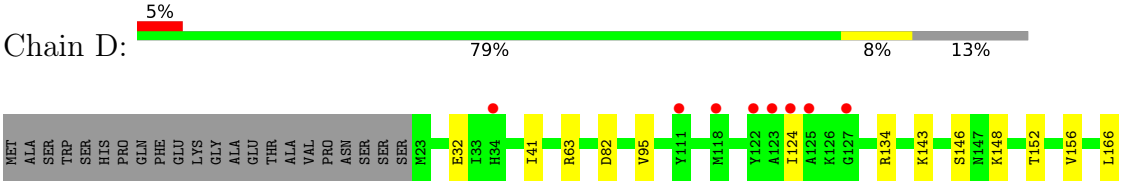
• Molecule 1: YtoQ

Chain C:



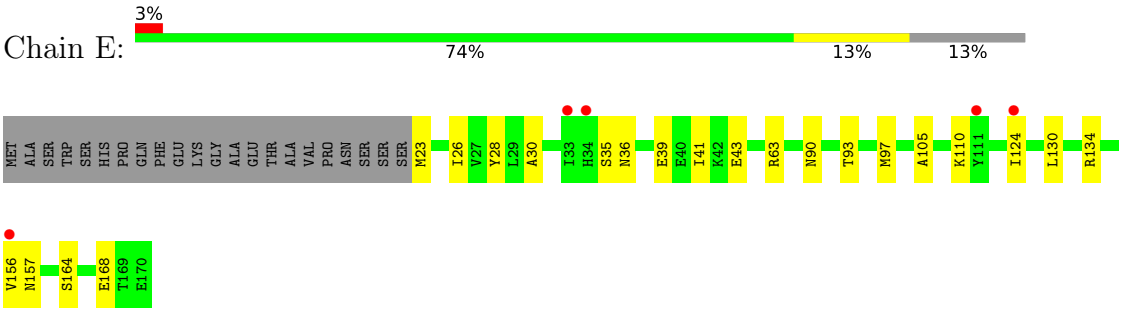
• Molecule 1: YtoQ

Chain D:



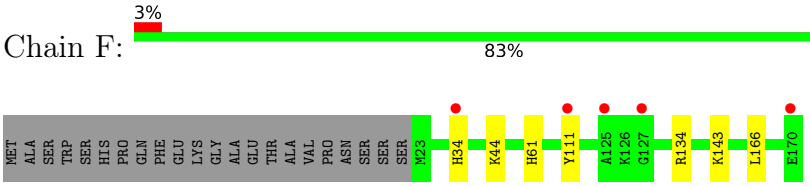
• Molecule 1: YtoQ

Chain E:



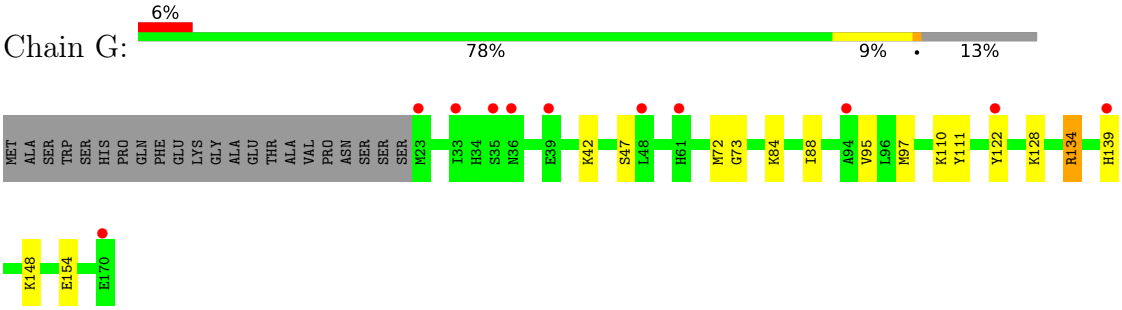
• Molecule 1: YtoQ

Chain F:



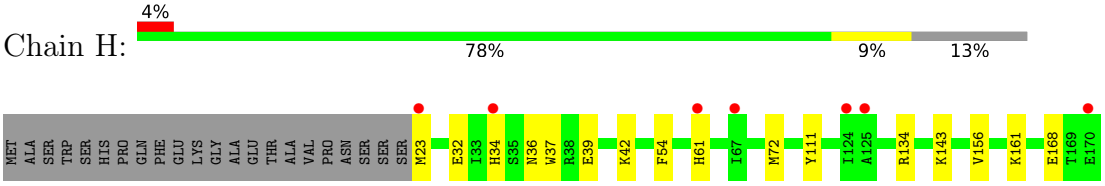
• Molecule 1: YtoQ

Chain G:



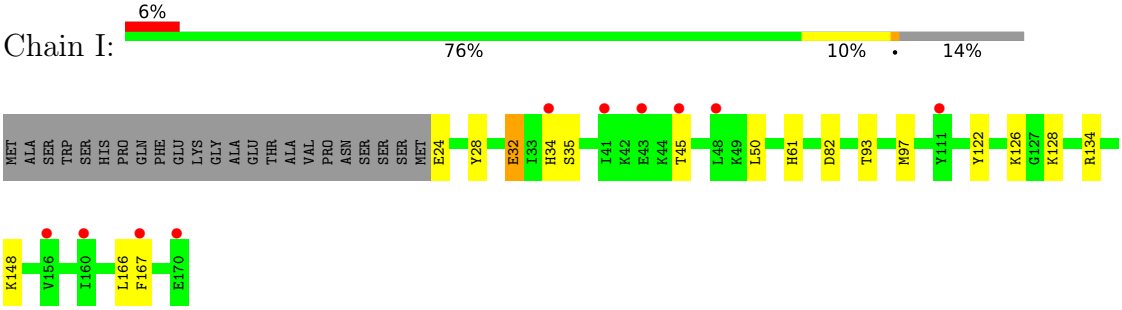
• Molecule 1: YtoQ

Chain H:



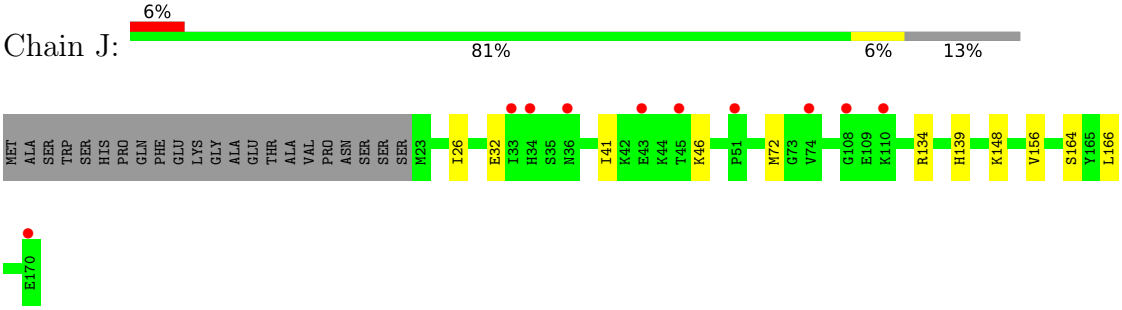
• Molecule 1: YtoQ

Chain I:



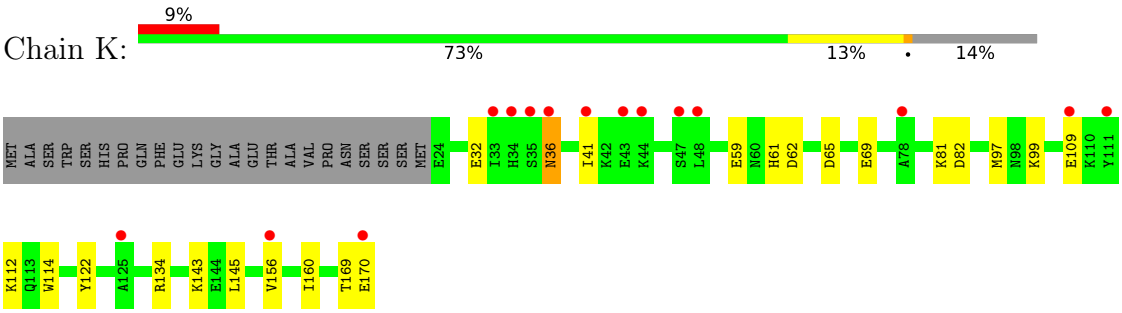
• Molecule 1: YtoQ

Chain J:



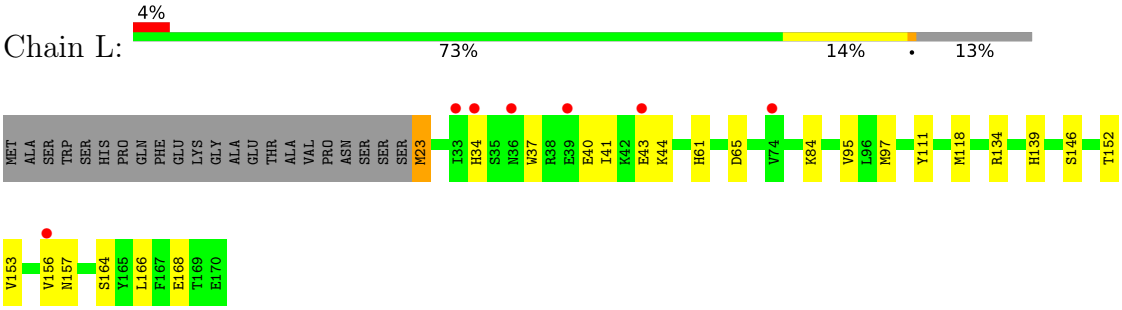
• Molecule 1: YtoQ

Chain K:



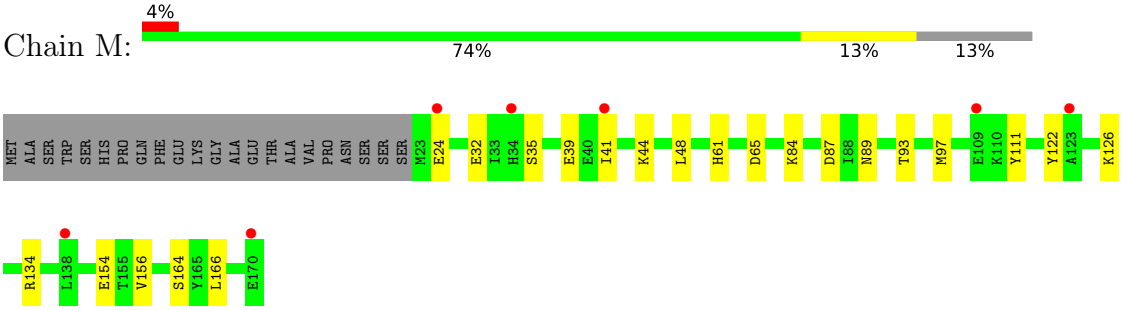
• Molecule 1: YtoQ

Chain L:



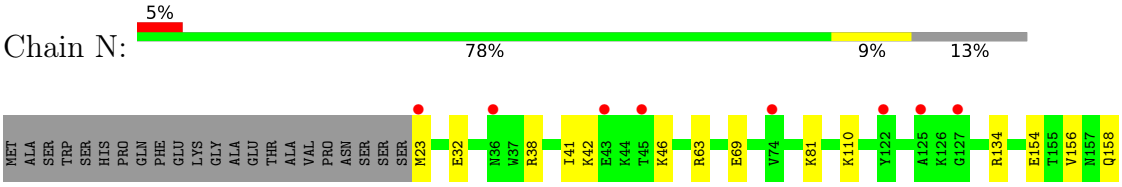
• Molecule 1: YtoQ

Chain M:



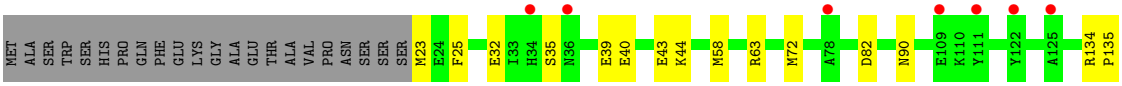
• Molecule 1: YtoQ

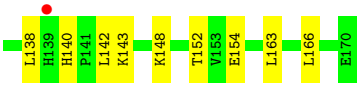
Chain N:



• Molecule 1: YtoQ

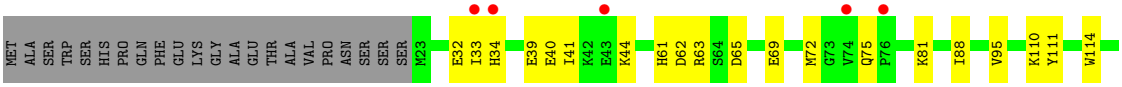
Chain O:





• Molecule 1: YtoQ

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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) 98.9 (49.45-2.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.227 , 0.268 0.226 , 0.265	Depositor DCC
R_{free} test set	8098 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	38576	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.42	0/1201	0.60	0/1623
1	B	0.50	0/1204	0.62	0/1626
1	C	0.47	0/1204	0.59	0/1626
1	D	0.47	0/1200	0.61	0/1622
1	E	0.49	0/1200	0.64	0/1622
1	F	0.46	0/1200	0.60	0/1621
1	G	0.49	0/1204	0.64	0/1626
1	H	0.52	0/1201	0.63	0/1623
1	I	0.40	0/1190	0.57	0/1610
1	J	0.43	0/1215	0.61	0/1641
1	K	0.41	0/1193	0.59	0/1613
1	L	0.46	0/1196	0.62	0/1617
1	M	0.41	0/1211	0.58	0/1637
1	N	0.44	0/1215	0.63	0/1641
1	O	0.48	0/1198	0.61	0/1618
1	P	0.44	0/1201	0.60	0/1621
All	All	0.46	0/19233	0.61	0/25987

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

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	9	0
1	B	1181	1186	1190	11	0
1	C	1181	1186	1190	15	0
1	D	1177	1177	1179	7	0
1	E	1177	1175	1179	11	0
1	F	1177	1182	1186	6	0
1	G	1181	1186	1190	14	0
1	H	1178	1179	1181	11	0
1	I	1167	1161	1163	13	0
1	J	1191	1192	1196	8	0
1	K	1170	1164	1172	21	0
1	L	1173	1166	1175	19	0
1	M	1187	1183	1185	11	0
1	N	1191	1192	1196	7	0
1	O	1176	1183	1185	18	0
1	P	1178	1179	1182	24	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
3	H	72	0	0	3	0
3	I	37	0	0	1	0
3	J	49	0	0	2	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	175	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.

All (175) 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
1:H:161:LYS:HE3	3:H:269:HOH:O	1.81	0.80
1:C:148:LYS:HE2	3:C:301:HOH:O	1.80	0.80
1:L:40:GLU:HA	1:L:43:GLU:OE1	1.83	0.79
1:G:42:LYS:HE3	3:G:202:HOH:O	1.85	0.76
1:L:34:HIS:ND1	1:L:111:TYR:CE2	2.54	0.74
1:K:112:LYS:NZ	3:K:201:HOH:O	2.20	0.74
1:K:41:ILE:CD1	1:K:160:ILE:HD11	2.18	0.73
1:I:82:ASP:HB2	1:J:139[B]:HIS:HE1	1.53	0.73
1:O:39:GLU:O	1:O:43:GLU:HG3	1.92	0.70
1:I:45:THR:HG23	1:I:50:LEU:HD12	1.74	0.70
1:M:44:LYS:O	1:M:48:LEU:HD12	1.93	0.68
1:O:90:ASN:HD22	1:P:147:ASN:HD22	1.40	0.68
1:I:82:ASP:HB2	1:J:139[B]:HIS:CE1	2.29	0.67
1:P:34:HIS:ND1	1:P:111:TYR:CZ	2.63	0.66
1:E:28:TYR:OH	1:E:93:THR:HG22	1.96	0.66
1:E:36:ASN:OD1	1:E:39:GLU:HG2	1.96	0.66
1:C:28:TYR:OH	1:C:93:THR:HG22	1.97	0.65
1:F:34:HIS:ND1	1:F:111:TYR:CZ	2.65	0.65
1:P:69:GLU:HG3	1:P:81:LYS:HG3	1.81	0.63
1:K:143:LYS:NZ	3:K:203:HOH:O	2.28	0.63
1:K:169:THR:OG1	1:K:170:GLU:OE1	2.15	0.62
1:F:34:HIS:ND1	1:F:111:TYR:OH	2.32	0.62
1:D:95:VAL:HG11	1:J:166:LEU:HD21	1.82	0.61
1:D:166:LEU:HD21	1:G:95:VAL:HG11	1.84	0.60
1:K:112:LYS:HD2	1:K:114:TRP:CH2	2.38	0.59
1:C:148:LYS:CE	3:C:301:HOH:O	2.44	0.58
1:B:36:ASN:OD1	1:B:39:GLU:CG	2.51	0.58
1:G:42:LYS:CE	3:G:202:HOH:O	2.48	0.58
1:E:124:ILE:HD11	1:E:130:LEU:HD23	1.86	0.57
1:B:72:MET:HE1	1:L:153:VAL:HG12	1.87	0.57
1:K:99:LYS:NZ	3:K:204:HOH:O	2.36	0.57
1:H:37:TRP:HA	3:H:207:HOH:O	2.04	0.57
1:O:135:PRO:HG2	1:O:138:LEU:HD12	1.85	0.57
1:B:23:MET:SD	1:E:26:ILE:HD13	2.45	0.56
1:I:97:MET:HG2	1:I:122:TYR:CE2	2.40	0.56
1:O:90:ASN:HD22	1:P:147:ASN:ND2	2.03	0.56
1:J:72:MET:HE1	1:O:152:THR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:89:ASN:O	1:M:93:THR:HG23	2.07	0.55
1:A:134:ARG:HH21	1:A:139:HIS:CD2	2.25	0.55
1:C:148:LYS:NZ	3:C:301:HOH:O	2.39	0.55
1:L:44:LYS:HE2	1:L:157:ASN:OD1	2.07	0.54
1:J:41:ILE:HG12	1:J:156:VAL:HG13	1.89	0.54
1:K:160:ILE:HD13	1:K:160:ILE:N	2.20	0.54
1:K:41:ILE:HD11	1:K:156:VAL:HG13	1.85	0.54
1:L:61:HIS:O	1:L:65:ASP:OD2	2.26	0.53
1:J:26:ILE:HD12	3:J:205:HOH:O	2.06	0.53
1:H:72:MET:HE1	1:P:153:VAL:HG12	1.91	0.53
1:O:148:LYS:HE3	1:P:118:MET:SD	2.49	0.53
1:B:168:GLU:HG2	1:E:63:ARG:HH12	1.74	0.52
1:C:63:ARG:NH1	1:H:168:GLU:OE1	2.37	0.52
1:C:26:ILE:HD13	1:H:23:MET:HE2	1.90	0.52
1:K:145:LEU:HD13	1:L:118:MET:HG3	1.91	0.52
1:O:58:MET:HE3	1:O:63:ARG:HG2	1.90	0.51
1:L:41:ILE:HG13	1:L:156:VAL:HG13	1.93	0.51
1:G:42:LYS:NZ	3:G:202:HOH:O	2.43	0.51
1:B:72:MET:CE	1:L:153:VAL:HG12	2.41	0.50
1:G:97:MET:HG2	1:G:122:TYR:CE1	2.46	0.50
1:L:95:VAL:HG11	1:M:166:LEU:HD21	1.92	0.50
1:I:28:TYR:HH	1:I:93:THR:HG22	1.70	0.50
1:K:61:HIS:NE2	1:K:65:ASP:OD2	2.43	0.50
1:H:34:HIS:CE1	1:H:61:HIS:CE1	2.99	0.50
3:A:203:HOH:O	1:K:99:LYS:NZ	2.44	0.50
1:C:36:ASN:OD1	1:C:39:GLU:HG3	2.12	0.50
1:O:140:HIS:CE1	1:O:143:LYS:HE2	2.47	0.50
1:B:26:ILE:HD13	1:L:23:MET:HE2	1.94	0.49
1:M:61:HIS:CE1	1:M:65:ASP:OD2	2.65	0.49
1:P:61:HIS:O	1:P:65:ASP:OD1	2.30	0.49
1:G:97:MET:HG3	1:G:128:LYS:HE3	1.95	0.49
1:C:139:HIS:CD2	1:D:82:ASP:OD2	2.65	0.49
1:D:41:ILE:HG12	1:D:156:VAL:HG13	1.94	0.48
1:K:169:THR:OG1	1:K:170:GLU:CD	2.51	0.48
1:P:34:HIS:CE1	1:P:111:TYR:CE1	3.01	0.48
1:A:134:ARG:HH21	1:A:139:HIS:HD2	1.60	0.48
1:E:90:ASN:HA	1:E:93:THR:OG1	2.14	0.48
1:H:36:ASN:OD1	1:H:39:GLU:OE1	2.31	0.48
1:M:97:MET:HG2	1:M:122:TYR:CE2	2.49	0.48
1:L:40:GLU:OE2	1:L:44:LYS:NZ	2.46	0.48
1:A:40:GLU:OE2	1:A:44:LYS:NZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:LYS:NZ	3:M:202:HOH:O	2.35	0.47
1:B:95:VAL:HG11	1:L:166:LEU:HD21	1.94	0.47
1:E:164:SER:O	1:E:168:GLU:HG3	2.14	0.47
1:F:34:HIS:HE1	3:F:225:HOH:O	1.96	0.47
1:G:134:ARG:HH21	1:G:139:HIS:CD2	2.32	0.47
1:O:140:HIS:CE1	1:P:65:ASP:OD2	2.68	0.47
1:D:146:SER:HB2	1:D:152:THR:OG1	2.14	0.47
1:O:40:GLU:OE2	1:O:44:LYS:NZ	2.45	0.47
1:K:82:ASP:OD2	1:L:139:HIS:NE2	2.47	0.47
1:M:41:ILE:HG12	1:M:156:VAL:HG13	1.96	0.47
1:J:148:LYS:NZ	3:J:203:HOH:O	2.48	0.47
1:O:23:MET:HG3	1:O:25:PHE:CE1	2.50	0.47
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.81	0.46
1:M:48:LEU:HD22	1:M:164:SER:OG	2.15	0.46
1:C:124:ILE:HD13	1:C:148:LYS:HB2	1.97	0.46
1:I:167:PHE:CD1	1:I:167:PHE:N	2.83	0.46
1:K:97:MET:HG2	1:K:122:TYR:CE1	2.50	0.46
1:K:59:GLU:HB2	3:K:232:HOH:O	2.16	0.46
1:P:33:ILE:HD11	1:P:61:HIS:HA	1.98	0.45
1:C:102:PHE:HB2	1:C:129:PRO:O	2.17	0.45
1:P:110:LYS:HB2	1:P:111:TYR:CE2	2.51	0.45
1:A:69:GLU:O	1:A:72:MET:O	2.34	0.45
1:M:111:TYR:HB3	3:M:236:HOH:O	2.16	0.45
1:A:163:LEU:O	1:A:166:LEU:HB2	2.16	0.45
1:K:69:GLU:HG3	1:K:81:LYS:HG3	1.98	0.45
1:N:154:GLU:N	1:N:158:GLN:OE1	2.50	0.45
1:E:41:ILE:HG13	1:E:156:VAL:HG13	1.98	0.45
1:C:72:MET:HE2	1:C:84:LYS:HB3	1.99	0.44
1:G:134:ARG:HH21	1:G:139:HIS:HD2	1.65	0.44
1:B:110:LYS:HA	1:B:110:LYS:HD3	1.80	0.44
1:E:30:ALA:O	1:E:105:ALA:HA	2.17	0.44
1:G:84:LYS:HA	1:G:84:LYS:HD3	1.77	0.44
1:G:110:LYS:HG2	1:G:111:TYR:CE2	2.53	0.44
1:O:135:PRO:CG	1:O:138:LEU:HD12	2.47	0.44
1:I:166:LEU:HB3	1:I:167:PHE:CD1	2.52	0.44
1:M:84:LYS:O	1:M:87:ASP:HB2	2.18	0.44
1:B:92:ARG:HA	1:L:166:LEU:CD1	2.48	0.44
1:E:93:THR:O	1:E:97:MET:HB2	2.17	0.44
1:P:63:ARG:HH11	1:P:63:ARG:HG2	1.81	0.44
1:A:139:HIS:HB3	3:B:347:HOH:O	2.18	0.44
1:B:41:ILE:HG12	1:B:156:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:164:SER:OG	1:L:168:GLU:OE2	2.31	0.44
1:C:90:ASN:HA	1:C:93:THR:OG1	2.18	0.43
1:H:34:HIS:CD2	1:H:111:TYR:CZ	3.06	0.43
1:A:44:LYS:O	1:A:48:LEU:HD23	2.18	0.43
1:C:39:GLU:O	1:C:43:GLU:OE1	2.35	0.43
1:G:110:LYS:HG2	1:G:111:TYR:CD2	2.53	0.43
1:I:97:MET:HG3	1:I:128:LYS:HE3	2.00	0.43
1:N:38:ARG:O	1:N:42:LYS:HG3	2.19	0.43
1:P:69:GLU:OE1	1:P:75:GLN:N	2.50	0.43
1:I:166:LEU:HD21	1:P:95:VAL:HG11	2.01	0.43
1:P:40:GLU:OE2	1:P:44:LYS:NZ	2.51	0.43
1:N:63:ARG:HG2	1:N:63:ARG:HH11	1.84	0.43
1:N:69:GLU:HG3	1:N:81:LYS:HG3	2.00	0.43
1:B:36:ASN:CG	1:B:39:GLU:CG	2.88	0.42
1:I:34:HIS:NE2	1:I:61:HIS:CE1	2.86	0.42
1:K:61:HIS:CE1	1:K:65:ASP:OD2	2.72	0.42
1:O:72:MET:HE2	1:O:72:MET:HB3	1.92	0.42
1:I:126:LYS:NZ	3:I:204:HOH:O	2.51	0.42
1:L:37:TRP:CE3	1:L:41:ILE:CD1	3.03	0.42
1:O:163:LEU:O	1:O:166:LEU:HB2	2.20	0.42
1:A:135:PRO:HD2	1:A:138:LEU:HD12	2.02	0.42
1:O:142:LEU:HG	1:P:114:TRP:CE3	2.54	0.42
1:P:148:LYS:HA	1:P:148:LYS:HD2	1.90	0.42
1:N:46:LYS:HB3	1:N:46:LYS:HE3	1.65	0.42
1:H:156:VAL:HB	3:H:236:HOH:O	2.19	0.42
1:A:95:VAL:HG11	1:F:166:LEU:HD21	2.01	0.42
1:G:148:LYS:HA	1:G:148:LYS:HD2	1.83	0.42
1:I:32:GLU:OE2	1:I:35:SER:HB3	2.19	0.42
1:J:72:MET:HE2	1:J:72:MET:HB3	1.88	0.42
1:P:72:MET:HE1	1:P:88:ILE:HD11	2.02	0.42
1:G:72:MET:CE	1:G:88:ILE:HD11	2.49	0.41
1:F:44:LYS:HE2	1:G:73:GLY:HA3	2.01	0.41
1:F:34:HIS:NE2	1:F:61:HIS:ND1	2.69	0.41
1:O:140:HIS:HE1	1:P:65:ASP:OD2	2.02	0.41
1:O:82:ASP:OD2	1:P:140:HIS:CD2	2.74	0.41
1:H:42:LYS:HG2	1:H:54:PHE:CD2	2.56	0.41
1:E:157:ASN:N	3:E:206:HOH:O	2.53	0.41
1:N:163:LEU:O	1:N:166:LEU:HB2	2.20	0.41
1:P:41:ILE:HG12	1:P:156:VAL:HG13	2.03	0.41
1:P:63:ARG:HD2	1:P:63:ARG:HA	1.87	0.41
1:C:26:ILE:HD13	1:H:23:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:154:GLU:N	1:O:154:GLU:OE1	2.54	0.41
1:P:140:HIS:O	1:P:143:LYS:HG2	2.20	0.41
1:N:41:ILE:HG12	1:N:156:VAL:HG13	2.03	0.41
1:D:124:ILE:HD13	1:D:148:LYS:HB2	2.03	0.40
1:L:84:LYS:HA	1:L:84:LYS:HD3	1.86	0.40
1:L:146:SER:HB2	1:L:152:THR:OG1	2.22	0.40
1:C:84:LYS:HA	1:C:84:LYS:HD3	1.79	0.40
1:L:41:ILE:HG13	1:L:156:VAL:CG1	2.51	0.40
1:K:36:ASN:HD22	1:K:36:ASN:H	1.69	0.40
1:P:110:LYS:CB	1:P:111:TYR:CD2	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	124 (97%)	4 (3%)	40	43
1	B	129/147 (88%)	126 (98%)	3 (2%)	50	55
1	C	129/147 (88%)	123 (95%)	6 (5%)	26	25
1	D	128/147 (87%)	125 (98%)	3 (2%)	50	55
1	E	128/147 (87%)	123 (96%)	5 (4%)	32	33
1	F	128/147 (87%)	126 (98%)	2 (2%)	62	69
1	G	129/147 (88%)	126 (98%)	3 (2%)	50	55
1	H	128/147 (87%)	125 (98%)	3 (2%)	50	55
1	I	126/147 (86%)	122 (97%)	4 (3%)	39	41
1	J	130/147 (88%)	126 (97%)	4 (3%)	40	43
1	K	127/147 (86%)	122 (96%)	5 (4%)	32	33
1	L	127/147 (86%)	124 (98%)	3 (2%)	49	53
1	M	129/147 (88%)	124 (96%)	5 (4%)	32	33
1	N	130/147 (88%)	126 (97%)	4 (3%)	40	43
1	O	128/147 (87%)	125 (98%)	3 (2%)	50	55
1	P	128/147 (87%)	122 (95%)	6 (5%)	26	25
All	All	2052/2352 (87%)	1989 (97%)	63 (3%)	40	43

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	48	LEU
1	A	72	MET
1	A	134	ARG
1	B	134	ARG
1	B	143	LYS
1	B	168	GLU
1	C	35	SER
1	C	46	LYS
1	C	47	SER
1	C	62	ASP
1	C	134	ARG
1	C	148	LYS
1	D	32	GLU
1	D	134	ARG
1	D	143	LYS
1	E	23	MET
1	E	35	SER
1	E	43	GLU
1	E	110	LYS
1	E	134	ARG
1	F	134	ARG
1	F	143	LYS
1	G	47	SER
1	G	134	ARG
1	G	154	GLU
1	H	32	GLU
1	H	134	ARG
1	H	143	LYS
1	I	24	GLU
1	I	32	GLU
1	I	134	ARG
1	I	148	LYS
1	J	32	GLU
1	J	46	LYS
1	J	134	ARG
1	J	164	SER
1	K	32	GLU
1	K	36	ASN
1	K	62	ASP
1	K	109	GLU
1	K	134	ARG

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Mol	Chain	Res	Type
1	L	23	MET
1	L	97	MET
1	L	134	ARG
1	M	32	GLU
1	M	35	SER
1	M	39	GLU
1	M	134	ARG
1	M	154	GLU
1	N	23	MET
1	N	32	GLU
1	N	110	LYS
1	N	134	ARG
1	O	32	GLU
1	O	35	SER
1	O	134	ARG
1	P	32	GLU
1	P	39	GLU
1	P	62	ASP
1	P	134	ARG
1	P	146	SER
1	P	164	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	139	HIS
1	D	75	GLN
1	G	139	HIS
1	H	34	HIS
1	H	61	HIS
1	I	61	HIS
1	K	36	ASN
1	K	75	GLN
1	K	139	HIS
1	N	75	GLN
1	P	140	HIS
1	P	147	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

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	B	201	-	4,4,4	0.47	0	6,6,6	0.10	0
2	SO4	C	201	-	4,4,4	0.42	0	6,6,6	0.06	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

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^{th} 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	148/170 (87%)	0.61	10 (6%) 17 21	26, 37, 57, 67	0
1	B	148/170 (87%)	0.56	5 (3%) 45 51	24, 34, 52, 61	1 (0%)
1	C	148/170 (87%)	0.65	10 (6%) 17 21	25, 36, 55, 65	0
1	D	148/170 (87%)	0.64	9 (6%) 21 26	26, 37, 54, 70	0
1	E	148/170 (87%)	0.60	5 (3%) 45 51	25, 37, 54, 65	0
1	F	148/170 (87%)	0.60	5 (3%) 45 51	25, 35, 51, 69	0
1	G	148/170 (87%)	0.62	11 (7%) 14 18	26, 36, 56, 67	0
1	H	148/170 (87%)	0.54	7 (4%) 31 37	24, 33, 50, 62	0
1	I	147/170 (86%)	0.71	10 (6%) 17 21	28, 42, 62, 72	0
1	J	148/170 (87%)	0.64	10 (6%) 17 21	26, 41, 61, 75	0
1	K	147/170 (86%)	0.72	15 (10%) 6 8	30, 44, 62, 76	0
1	L	148/170 (87%)	0.54	7 (4%) 31 37	27, 43, 61, 69	2 (1%)
1	M	148/170 (87%)	0.61	7 (4%) 31 37	29, 40, 63, 71	0
1	N	148/170 (87%)	0.47	9 (6%) 21 26	27, 40, 58, 62	1 (0%)
1	O	148/170 (87%)	0.56	8 (5%) 25 31	30, 43, 61, 68	0
1	P	148/170 (87%)	0.59	6 (4%) 37 43	28, 42, 62, 68	2 (1%)
All	All	2366/2720 (86%)	0.60	134 (5%) 23 29	24, 39, 59, 76	6 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	111	TYR	4.8
1	P	74	VAL	4.7
1	J	108	GLY	4.7
1	F	34	HIS	4.6
1	E	34	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	34	HIS	4.0
1	A	34	HIS	4.0
1	P	170	GLU	3.9
1	O	36	ASN	3.8
1	I	167	PHE	3.8
1	C	34	HIS	3.8
1	D	111	TYR	3.7
1	F	125	ALA	3.6
1	K	36	ASN	3.6
1	L	39	GLU	3.6
1	K	170	GLU	3.6
1	P	76	PRO	3.6
1	D	125	ALA	3.5
1	J	170	GLU	3.5
1	C	33	ILE	3.5
1	F	111	TYR	3.5
1	E	111	TYR	3.5
1	K	34	HIS	3.4
1	D	34	HIS	3.4
1	I	34	HIS	3.4
1	A	33	ILE	3.4
1	K	41	ILE	3.3
1	K	78	ALA	3.3
1	N	170	GLU	3.3
1	I	41	ILE	3.2
1	O	34	HIS	3.2
1	I	48	LEU	3.2
1	G	33	ILE	3.2
1	K	33	ILE	3.2
1	D	170	GLU	3.2
1	I	160	ILE	3.1
1	J	36	ASN	3.0
1	G	61	HIS	3.0
1	K	47	SER	3.0
1	C	124	ILE	2.9
1	M	24	GLU	2.9
1	A	36	ASN	2.9
1	C	36	ASN	2.9
1	G	23	MET	2.9
1	K	109	GLU	2.9
1	J	51	PRO	2.8
1	L	156	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	43	GLU	2.8
1	H	34	HIS	2.8
1	M	138	LEU	2.7
1	M	123	ALA	2.7
1	K	43	GLU	2.7
1	E	33	ILE	2.7
1	B	170	GLU	2.7
1	G	35	SER	2.7
1	I	170	GLU	2.7
1	E	124	ILE	2.7
1	O	125	ALA	2.7
1	A	94	ALA	2.6
1	N	36	ASN	2.6
1	N	45	THR	2.6
1	J	33	ILE	2.6
1	N	127	GLY	2.6
1	G	48	LEU	2.6
1	K	44	LYS	2.6
1	I	45	THR	2.6
1	M	170	GLU	2.6
1	C	125	ALA	2.5
1	C	43	GLU	2.5
1	G	170	GLU	2.5
1	P	43	GLU	2.5
1	D	118	MET	2.5
1	A	111	TYR	2.5
1	D	122	TYR	2.5
1	M	109	GLU	2.5
1	D	127	GLY	2.5
1	A	125	ALA	2.5
1	B	125	ALA	2.5
1	H	61	HIS	2.5
1	I	43	GLU	2.5
1	L	43	GLU	2.5
1	C	97	MET	2.5
1	L	34	HIS	2.5
1	O	109	GLU	2.5
1	F	127	GLY	2.4
1	P	33	ILE	2.4
1	L	74	VAL	2.4
1	N	74	VAL	2.4
1	I	156	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	125	ALA	2.4
1	N	23	MET	2.4
1	E	156	VAL	2.4
1	B	169	THR	2.4
1	M	41	ILE	2.4
1	D	123	ALA	2.3
1	O	78	ALA	2.3
1	D	124	ILE	2.3
1	O	122	TYR	2.3
1	H	170	GLU	2.3
1	B	123	ALA	2.3
1	H	124	ILE	2.3
1	J	110	LYS	2.3
1	G	39	GLU	2.3
1	K	35	SER	2.3
1	H	125	ALA	2.3
1	K	156	VAL	2.3
1	B	124	ILE	2.2
1	C	122	TYR	2.2
1	L	36	ASN	2.2
1	A	95	VAL	2.2
1	K	48	LEU	2.2
1	G	122	TYR	2.2
1	O	111	TYR	2.2
1	J	43	GLU	2.1
1	A	122	TYR	2.1
1	H	67	ILE	2.1
1	F	170	GLU	2.1
1	J	34	HIS	2.1
1	L	33	ILE	2.1
1	N	122	TYR	2.1
1	A	39	GLU	2.1
1	O	139	HIS	2.1
1	P	34	HIS	2.1
1	A	24	GLU	2.1
1	G	36	ASN	2.1
1	C	123	ALA	2.1
1	G	94	ALA	2.0
1	J	45	THR	2.0
1	J	74	VAL	2.0
1	I	111	TYR	2.0
1	H	23	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	139	HIS	2.0
1	N	125	ALA	2.0
1	C	127	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	SO4	C	201	5/5	0.82	0.47	75,86,92,108	0
2	SO4	B	201	5/5	0.89	0.19	47,59,63,76	0

6.5 Other polymers (i)

There are no such residues in this entry.