



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2025 – 04:52 PM EST

PDB ID : 9BT6  
Title : Crystal structure of Chorismate Mutase from Mycobacterium tuberculosis in complex with the cyclic peptide inhibitor L2.1 (monoclinic P form)  
Authors : Liu, L.; Lovell, S.; Battaile, K.P.; Inglese, J.  
Deposited on : 2024-05-14  
Resolution : 2.80 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 : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

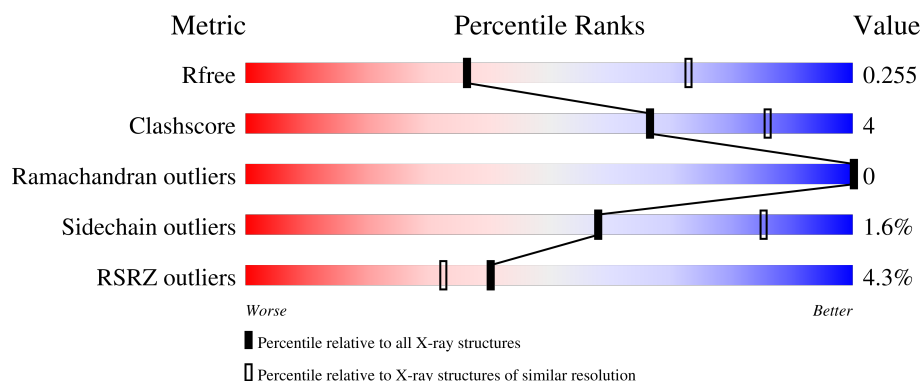
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	205	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>21%</div> </div> </div>
1	B	205	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>.</div> <div>21%</div> </div> </div>
1	C	205	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>6%</div> <div>22%</div> </div> </div>
1	D	205	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>5%</div> <div>22%</div> </div> </div>
1	E	205	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>9%</div> <div>22%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	205	
1	G	205	
1	H	205	
2	a	14	
2	b	14	
2	c	14	
2	d	14	
2	e	14	
2	f	14	
2	g	14	
2	h	14	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11296 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 Secreted chorismate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	B	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	C	159	Total	C	N	O	S	0	0	0
			1257	778	229	247	3			
1	D	160	Total	C	N	O	S	0	0	0
			1262	781	230	248	3			
1	E	160	Total	C	N	O	S	0	0	0
			1262	781	230	248	3			
1	F	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	G	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	H	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	-	expression tag	UNP P9WIB9
A	201	LEU	-	expression tag	UNP P9WIB9
A	202	ASN	-	expression tag	UNP P9WIB9
A	203	ASP	-	expression tag	UNP P9WIB9
A	204	ILE	-	expression tag	UNP P9WIB9
A	205	PHE	-	expression tag	UNP P9WIB9
A	206	GLU	-	expression tag	UNP P9WIB9
A	207	ALA	-	expression tag	UNP P9WIB9
A	208	GLN	-	expression tag	UNP P9WIB9
A	209	LYS	-	expression tag	UNP P9WIB9
A	210	ILE	-	expression tag	UNP P9WIB9
A	211	GLU	-	expression tag	UNP P9WIB9
A	212	TRP	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	213	HIS	-	expression tag	UNP P9WIB9
A	214	GLU	-	expression tag	UNP P9WIB9
A	215	SER	-	expression tag	UNP P9WIB9
A	216	SER	-	expression tag	UNP P9WIB9
A	217	GLY	-	expression tag	UNP P9WIB9
A	218	LEU	-	expression tag	UNP P9WIB9
A	219	VAL	-	expression tag	UNP P9WIB9
A	220	PRO	-	expression tag	UNP P9WIB9
A	221	ARG	-	expression tag	UNP P9WIB9
A	222	GLY	-	expression tag	UNP P9WIB9
A	223	SER	-	expression tag	UNP P9WIB9
A	224	ALA	-	expression tag	UNP P9WIB9
A	225	ALA	-	expression tag	UNP P9WIB9
A	226	GLY	-	expression tag	UNP P9WIB9
A	227	HIS	-	expression tag	UNP P9WIB9
A	228	HIS	-	expression tag	UNP P9WIB9
A	229	HIS	-	expression tag	UNP P9WIB9
A	230	HIS	-	expression tag	UNP P9WIB9
A	231	HIS	-	expression tag	UNP P9WIB9
A	232	HIS	-	expression tag	UNP P9WIB9
A	233	HIS	-	expression tag	UNP P9WIB9
A	234	HIS	-	expression tag	UNP P9WIB9
A	235	HIS	-	expression tag	UNP P9WIB9
A	236	HIS	-	expression tag	UNP P9WIB9
A	237	GLU	-	expression tag	UNP P9WIB9
A	238	LEU	-	expression tag	UNP P9WIB9
B	200	GLY	-	expression tag	UNP P9WIB9
B	201	LEU	-	expression tag	UNP P9WIB9
B	202	ASN	-	expression tag	UNP P9WIB9
B	203	ASP	-	expression tag	UNP P9WIB9
B	204	ILE	-	expression tag	UNP P9WIB9
B	205	PHE	-	expression tag	UNP P9WIB9
B	206	GLU	-	expression tag	UNP P9WIB9
B	207	ALA	-	expression tag	UNP P9WIB9
B	208	GLN	-	expression tag	UNP P9WIB9
B	209	LYS	-	expression tag	UNP P9WIB9
B	210	ILE	-	expression tag	UNP P9WIB9
B	211	GLU	-	expression tag	UNP P9WIB9
B	212	TRP	-	expression tag	UNP P9WIB9
B	213	HIS	-	expression tag	UNP P9WIB9
B	214	GLU	-	expression tag	UNP P9WIB9
B	215	SER	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	216	SER	-	expression tag	UNP P9WIB9
B	217	GLY	-	expression tag	UNP P9WIB9
B	218	LEU	-	expression tag	UNP P9WIB9
B	219	VAL	-	expression tag	UNP P9WIB9
B	220	PRO	-	expression tag	UNP P9WIB9
B	221	ARG	-	expression tag	UNP P9WIB9
B	222	GLY	-	expression tag	UNP P9WIB9
B	223	SER	-	expression tag	UNP P9WIB9
B	224	ALA	-	expression tag	UNP P9WIB9
B	225	ALA	-	expression tag	UNP P9WIB9
B	226	GLY	-	expression tag	UNP P9WIB9
B	227	HIS	-	expression tag	UNP P9WIB9
B	228	HIS	-	expression tag	UNP P9WIB9
B	229	HIS	-	expression tag	UNP P9WIB9
B	230	HIS	-	expression tag	UNP P9WIB9
B	231	HIS	-	expression tag	UNP P9WIB9
B	232	HIS	-	expression tag	UNP P9WIB9
B	233	HIS	-	expression tag	UNP P9WIB9
B	234	HIS	-	expression tag	UNP P9WIB9
B	235	HIS	-	expression tag	UNP P9WIB9
B	236	HIS	-	expression tag	UNP P9WIB9
B	237	GLU	-	expression tag	UNP P9WIB9
B	238	LEU	-	expression tag	UNP P9WIB9
C	200	GLY	-	expression tag	UNP P9WIB9
C	201	LEU	-	expression tag	UNP P9WIB9
C	202	ASN	-	expression tag	UNP P9WIB9
C	203	ASP	-	expression tag	UNP P9WIB9
C	204	ILE	-	expression tag	UNP P9WIB9
C	205	PHE	-	expression tag	UNP P9WIB9
C	206	GLU	-	expression tag	UNP P9WIB9
C	207	ALA	-	expression tag	UNP P9WIB9
C	208	GLN	-	expression tag	UNP P9WIB9
C	209	LYS	-	expression tag	UNP P9WIB9
C	210	ILE	-	expression tag	UNP P9WIB9
C	211	GLU	-	expression tag	UNP P9WIB9
C	212	TRP	-	expression tag	UNP P9WIB9
C	213	HIS	-	expression tag	UNP P9WIB9
C	214	GLU	-	expression tag	UNP P9WIB9
C	215	SER	-	expression tag	UNP P9WIB9
C	216	SER	-	expression tag	UNP P9WIB9
C	217	GLY	-	expression tag	UNP P9WIB9
C	218	LEU	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	219	VAL	-	expression tag	UNP P9WIB9
C	220	PRO	-	expression tag	UNP P9WIB9
C	221	ARG	-	expression tag	UNP P9WIB9
C	222	GLY	-	expression tag	UNP P9WIB9
C	223	SER	-	expression tag	UNP P9WIB9
C	224	ALA	-	expression tag	UNP P9WIB9
C	225	ALA	-	expression tag	UNP P9WIB9
C	226	GLY	-	expression tag	UNP P9WIB9
C	227	HIS	-	expression tag	UNP P9WIB9
C	228	HIS	-	expression tag	UNP P9WIB9
C	229	HIS	-	expression tag	UNP P9WIB9
C	230	HIS	-	expression tag	UNP P9WIB9
C	231	HIS	-	expression tag	UNP P9WIB9
C	232	HIS	-	expression tag	UNP P9WIB9
C	233	HIS	-	expression tag	UNP P9WIB9
C	234	HIS	-	expression tag	UNP P9WIB9
C	235	HIS	-	expression tag	UNP P9WIB9
C	236	HIS	-	expression tag	UNP P9WIB9
C	237	GLU	-	expression tag	UNP P9WIB9
C	238	LEU	-	expression tag	UNP P9WIB9
D	200	GLY	-	expression tag	UNP P9WIB9
D	201	LEU	-	expression tag	UNP P9WIB9
D	202	ASN	-	expression tag	UNP P9WIB9
D	203	ASP	-	expression tag	UNP P9WIB9
D	204	ILE	-	expression tag	UNP P9WIB9
D	205	PHE	-	expression tag	UNP P9WIB9
D	206	GLU	-	expression tag	UNP P9WIB9
D	207	ALA	-	expression tag	UNP P9WIB9
D	208	GLN	-	expression tag	UNP P9WIB9
D	209	LYS	-	expression tag	UNP P9WIB9
D	210	ILE	-	expression tag	UNP P9WIB9
D	211	GLU	-	expression tag	UNP P9WIB9
D	212	TRP	-	expression tag	UNP P9WIB9
D	213	HIS	-	expression tag	UNP P9WIB9
D	214	GLU	-	expression tag	UNP P9WIB9
D	215	SER	-	expression tag	UNP P9WIB9
D	216	SER	-	expression tag	UNP P9WIB9
D	217	GLY	-	expression tag	UNP P9WIB9
D	218	LEU	-	expression tag	UNP P9WIB9
D	219	VAL	-	expression tag	UNP P9WIB9
D	220	PRO	-	expression tag	UNP P9WIB9
D	221	ARG	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	222	GLY	-	expression tag	UNP P9WIB9
D	223	SER	-	expression tag	UNP P9WIB9
D	224	ALA	-	expression tag	UNP P9WIB9
D	225	ALA	-	expression tag	UNP P9WIB9
D	226	GLY	-	expression tag	UNP P9WIB9
D	227	HIS	-	expression tag	UNP P9WIB9
D	228	HIS	-	expression tag	UNP P9WIB9
D	229	HIS	-	expression tag	UNP P9WIB9
D	230	HIS	-	expression tag	UNP P9WIB9
D	231	HIS	-	expression tag	UNP P9WIB9
D	232	HIS	-	expression tag	UNP P9WIB9
D	233	HIS	-	expression tag	UNP P9WIB9
D	234	HIS	-	expression tag	UNP P9WIB9
D	235	HIS	-	expression tag	UNP P9WIB9
D	236	HIS	-	expression tag	UNP P9WIB9
D	237	GLU	-	expression tag	UNP P9WIB9
D	238	LEU	-	expression tag	UNP P9WIB9
E	200	GLY	-	expression tag	UNP P9WIB9
E	201	LEU	-	expression tag	UNP P9WIB9
E	202	ASN	-	expression tag	UNP P9WIB9
E	203	ASP	-	expression tag	UNP P9WIB9
E	204	ILE	-	expression tag	UNP P9WIB9
E	205	PHE	-	expression tag	UNP P9WIB9
E	206	GLU	-	expression tag	UNP P9WIB9
E	207	ALA	-	expression tag	UNP P9WIB9
E	208	GLN	-	expression tag	UNP P9WIB9
E	209	LYS	-	expression tag	UNP P9WIB9
E	210	ILE	-	expression tag	UNP P9WIB9
E	211	GLU	-	expression tag	UNP P9WIB9
E	212	TRP	-	expression tag	UNP P9WIB9
E	213	HIS	-	expression tag	UNP P9WIB9
E	214	GLU	-	expression tag	UNP P9WIB9
E	215	SER	-	expression tag	UNP P9WIB9
E	216	SER	-	expression tag	UNP P9WIB9
E	217	GLY	-	expression tag	UNP P9WIB9
E	218	LEU	-	expression tag	UNP P9WIB9
E	219	VAL	-	expression tag	UNP P9WIB9
E	220	PRO	-	expression tag	UNP P9WIB9
E	221	ARG	-	expression tag	UNP P9WIB9
E	222	GLY	-	expression tag	UNP P9WIB9
E	223	SER	-	expression tag	UNP P9WIB9
E	224	ALA	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	225	ALA	-	expression tag	UNP P9WIB9
E	226	GLY	-	expression tag	UNP P9WIB9
E	227	HIS	-	expression tag	UNP P9WIB9
E	228	HIS	-	expression tag	UNP P9WIB9
E	229	HIS	-	expression tag	UNP P9WIB9
E	230	HIS	-	expression tag	UNP P9WIB9
E	231	HIS	-	expression tag	UNP P9WIB9
E	232	HIS	-	expression tag	UNP P9WIB9
E	233	HIS	-	expression tag	UNP P9WIB9
E	234	HIS	-	expression tag	UNP P9WIB9
E	235	HIS	-	expression tag	UNP P9WIB9
E	236	HIS	-	expression tag	UNP P9WIB9
E	237	GLU	-	expression tag	UNP P9WIB9
E	238	LEU	-	expression tag	UNP P9WIB9
F	200	GLY	-	expression tag	UNP P9WIB9
F	201	LEU	-	expression tag	UNP P9WIB9
F	202	ASN	-	expression tag	UNP P9WIB9
F	203	ASP	-	expression tag	UNP P9WIB9
F	204	ILE	-	expression tag	UNP P9WIB9
F	205	PHE	-	expression tag	UNP P9WIB9
F	206	GLU	-	expression tag	UNP P9WIB9
F	207	ALA	-	expression tag	UNP P9WIB9
F	208	GLN	-	expression tag	UNP P9WIB9
F	209	LYS	-	expression tag	UNP P9WIB9
F	210	ILE	-	expression tag	UNP P9WIB9
F	211	GLU	-	expression tag	UNP P9WIB9
F	212	TRP	-	expression tag	UNP P9WIB9
F	213	HIS	-	expression tag	UNP P9WIB9
F	214	GLU	-	expression tag	UNP P9WIB9
F	215	SER	-	expression tag	UNP P9WIB9
F	216	SER	-	expression tag	UNP P9WIB9
F	217	GLY	-	expression tag	UNP P9WIB9
F	218	LEU	-	expression tag	UNP P9WIB9
F	219	VAL	-	expression tag	UNP P9WIB9
F	220	PRO	-	expression tag	UNP P9WIB9
F	221	ARG	-	expression tag	UNP P9WIB9
F	222	GLY	-	expression tag	UNP P9WIB9
F	223	SER	-	expression tag	UNP P9WIB9
F	224	ALA	-	expression tag	UNP P9WIB9
F	225	ALA	-	expression tag	UNP P9WIB9
F	226	GLY	-	expression tag	UNP P9WIB9
F	227	HIS	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	228	HIS	-	expression tag	UNP P9WIB9
F	229	HIS	-	expression tag	UNP P9WIB9
F	230	HIS	-	expression tag	UNP P9WIB9
F	231	HIS	-	expression tag	UNP P9WIB9
F	232	HIS	-	expression tag	UNP P9WIB9
F	233	HIS	-	expression tag	UNP P9WIB9
F	234	HIS	-	expression tag	UNP P9WIB9
F	235	HIS	-	expression tag	UNP P9WIB9
F	236	HIS	-	expression tag	UNP P9WIB9
F	237	GLU	-	expression tag	UNP P9WIB9
F	238	LEU	-	expression tag	UNP P9WIB9
G	200	GLY	-	expression tag	UNP P9WIB9
G	201	LEU	-	expression tag	UNP P9WIB9
G	202	ASN	-	expression tag	UNP P9WIB9
G	203	ASP	-	expression tag	UNP P9WIB9
G	204	ILE	-	expression tag	UNP P9WIB9
G	205	PHE	-	expression tag	UNP P9WIB9
G	206	GLU	-	expression tag	UNP P9WIB9
G	207	ALA	-	expression tag	UNP P9WIB9
G	208	GLN	-	expression tag	UNP P9WIB9
G	209	LYS	-	expression tag	UNP P9WIB9
G	210	ILE	-	expression tag	UNP P9WIB9
G	211	GLU	-	expression tag	UNP P9WIB9
G	212	TRP	-	expression tag	UNP P9WIB9
G	213	HIS	-	expression tag	UNP P9WIB9
G	214	GLU	-	expression tag	UNP P9WIB9
G	215	SER	-	expression tag	UNP P9WIB9
G	216	SER	-	expression tag	UNP P9WIB9
G	217	GLY	-	expression tag	UNP P9WIB9
G	218	LEU	-	expression tag	UNP P9WIB9
G	219	VAL	-	expression tag	UNP P9WIB9
G	220	PRO	-	expression tag	UNP P9WIB9
G	221	ARG	-	expression tag	UNP P9WIB9
G	222	GLY	-	expression tag	UNP P9WIB9
G	223	SER	-	expression tag	UNP P9WIB9
G	224	ALA	-	expression tag	UNP P9WIB9
G	225	ALA	-	expression tag	UNP P9WIB9
G	226	GLY	-	expression tag	UNP P9WIB9
G	227	HIS	-	expression tag	UNP P9WIB9
G	228	HIS	-	expression tag	UNP P9WIB9
G	229	HIS	-	expression tag	UNP P9WIB9
G	230	HIS	-	expression tag	UNP P9WIB9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	231	HIS	-	expression tag	UNP P9WIB9
G	232	HIS	-	expression tag	UNP P9WIB9
G	233	HIS	-	expression tag	UNP P9WIB9
G	234	HIS	-	expression tag	UNP P9WIB9
G	235	HIS	-	expression tag	UNP P9WIB9
G	236	HIS	-	expression tag	UNP P9WIB9
G	237	GLU	-	expression tag	UNP P9WIB9
G	238	LEU	-	expression tag	UNP P9WIB9
H	200	GLY	-	expression tag	UNP P9WIB9
H	201	LEU	-	expression tag	UNP P9WIB9
H	202	ASN	-	expression tag	UNP P9WIB9
H	203	ASP	-	expression tag	UNP P9WIB9
H	204	ILE	-	expression tag	UNP P9WIB9
H	205	PHE	-	expression tag	UNP P9WIB9
H	206	GLU	-	expression tag	UNP P9WIB9
H	207	ALA	-	expression tag	UNP P9WIB9
H	208	GLN	-	expression tag	UNP P9WIB9
H	209	LYS	-	expression tag	UNP P9WIB9
H	210	ILE	-	expression tag	UNP P9WIB9
H	211	GLU	-	expression tag	UNP P9WIB9
H	212	TRP	-	expression tag	UNP P9WIB9
H	213	HIS	-	expression tag	UNP P9WIB9
H	214	GLU	-	expression tag	UNP P9WIB9
H	215	SER	-	expression tag	UNP P9WIB9
H	216	SER	-	expression tag	UNP P9WIB9
H	217	GLY	-	expression tag	UNP P9WIB9
H	218	LEU	-	expression tag	UNP P9WIB9
H	219	VAL	-	expression tag	UNP P9WIB9
H	220	PRO	-	expression tag	UNP P9WIB9
H	221	ARG	-	expression tag	UNP P9WIB9
H	222	GLY	-	expression tag	UNP P9WIB9
H	223	SER	-	expression tag	UNP P9WIB9
H	224	ALA	-	expression tag	UNP P9WIB9
H	225	ALA	-	expression tag	UNP P9WIB9
H	226	GLY	-	expression tag	UNP P9WIB9
H	227	HIS	-	expression tag	UNP P9WIB9
H	228	HIS	-	expression tag	UNP P9WIB9
H	229	HIS	-	expression tag	UNP P9WIB9
H	230	HIS	-	expression tag	UNP P9WIB9
H	231	HIS	-	expression tag	UNP P9WIB9
H	232	HIS	-	expression tag	UNP P9WIB9
H	233	HIS	-	expression tag	UNP P9WIB9

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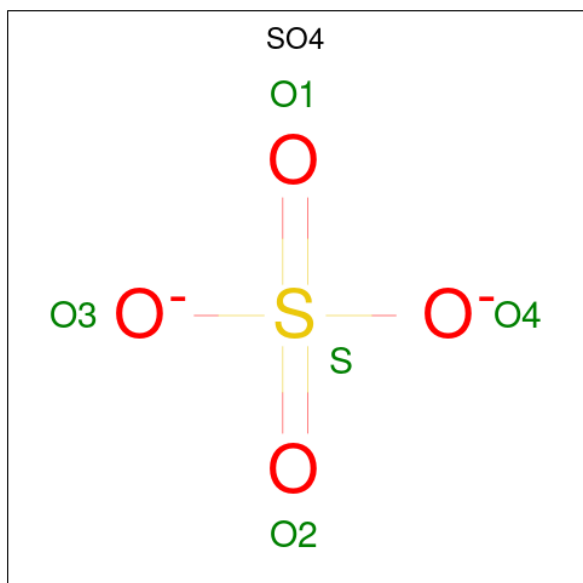
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Chain	Residue	Modelled	Actual	Comment	Reference
H	234	HIS	-	expression tag	UNP P9WIB9
H	235	HIS	-	expression tag	UNP P9WIB9
H	236	HIS	-	expression tag	UNP P9WIB9
H	237	GLU	-	expression tag	UNP P9WIB9
H	238	LEU	-	expression tag	UNP P9WIB9

- Molecule 2 is a protein called Peptide L2.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			
2	b	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			
2	c	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			
2	d	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			
2	e	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			
2	f	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			
2	g	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			
2	h	14	Total	C	N	O	S	0	0	0
			127	90	15	21	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

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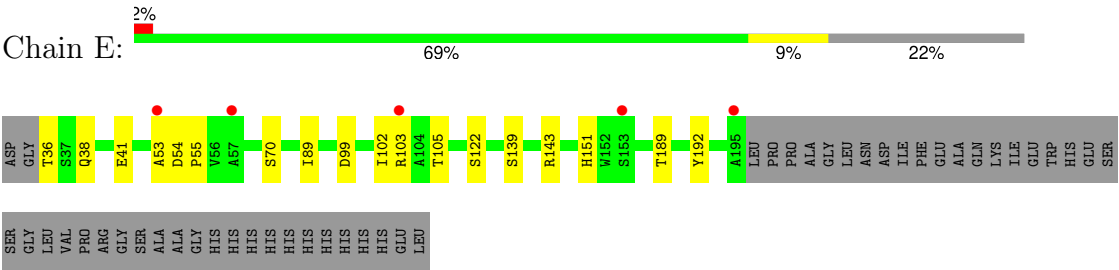
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	a	1	Total	O	S	0	0
			5	4	1		
3	b	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	d	1	Total	O	S	0	0
			5	4	1		
3	f	1	Total	O	S	0	0
			5	4	1		

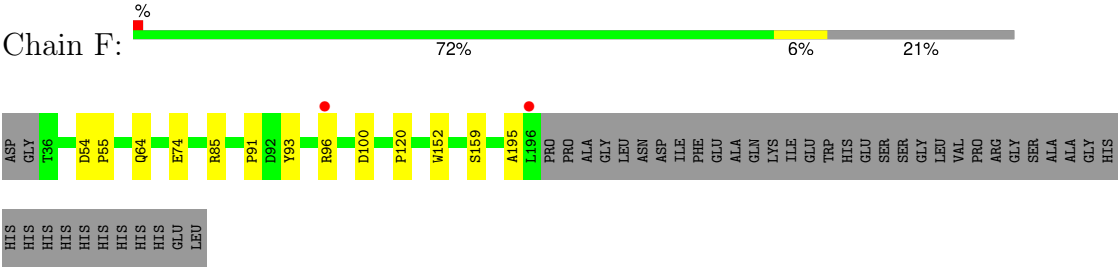
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	3	Total	O	0	0
			3	3		
4	D	1	Total	O	0	0
			1	1		
4	E	2	Total	O	0	0
			2	2		
4	G	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		

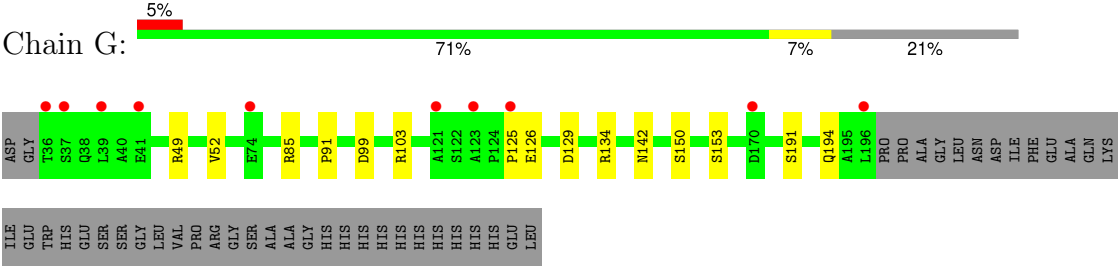




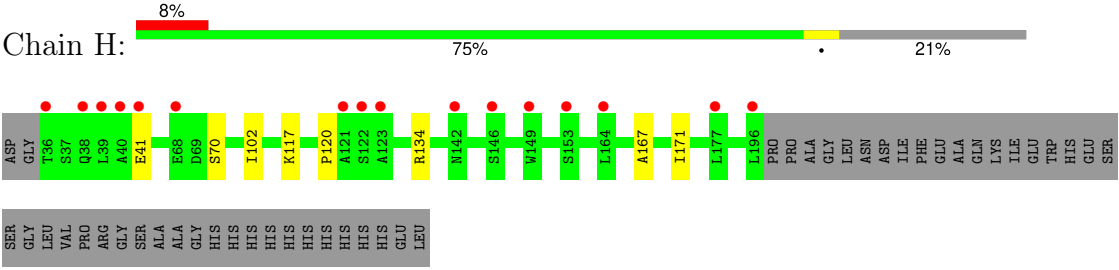
• Molecule 1: Secreted chorismate mutase



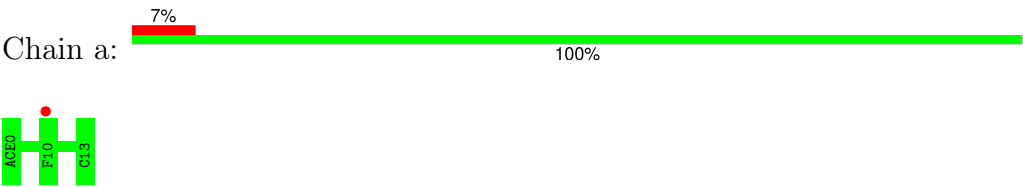
• Molecule 1: Secreted chorismate mutase



• Molecule 1: Secreted chorismate mutase



• Molecule 2: Peptide L2.1



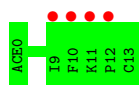
• Molecule 2: Peptide L2.1



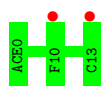




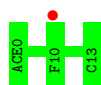
- Molecule 2: Peptide L2.1



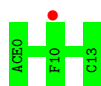
- Molecule 2: Peptide L2.1



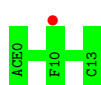
- Molecule 2: Peptide L2.1



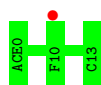
- Molecule 2: Peptide L2.1



- Molecule 2: Peptide L2.1



- Molecule 2: Peptide L2.1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.45Å 120.34Å 143.40Å 90.00° 95.32° 90.00°	Depositor
Resolution (Å)	142.79 – 2.80 142.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.9 (142.79-2.80) 93.0 (142.78-2.80)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.210 , 0.250 0.217 , 0.255	Depositor DCC
$R_{free}$ test set	2298 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11296	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	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 22.67 % 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 5.4407e-03. 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, ACE

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	0.31	0/1296	0.54	0/1764
1	B	0.33	0/1296	0.54	0/1764
1	C	0.27	0/1283	0.54	0/1746
1	D	0.30	0/1288	0.53	0/1753
1	E	0.29	0/1288	0.55	0/1753
1	F	0.31	0/1296	0.54	0/1764
1	G	0.31	0/1296	0.51	0/1764
1	H	0.29	0/1296	0.52	0/1764
2	a	0.43	0/131	0.59	0/178
2	b	0.39	0/131	0.59	0/178
2	c	0.38	0/131	0.70	0/178
2	d	0.53	0/131	0.67	0/178
2	e	0.63	0/131	0.63	0/178
2	f	0.54	0/131	0.54	0/178
2	g	0.41	0/131	0.58	0/178
2	h	0.41	0/131	0.51	0/178
All	All	0.32	0/11387	0.54	0/15496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1270	0	1233	8	0
1	B	1270	0	1233	2	0
1	C	1257	0	1217	7	0
1	D	1262	0	1222	6	0
1	E	1262	0	1222	11	0
1	F	1270	0	1233	9	0
1	G	1270	0	1233	10	0
1	H	1270	0	1233	4	0
2	a	127	0	119	0	0
2	b	127	0	119	0	0
2	c	127	0	119	0	0
2	d	127	0	119	0	0
2	e	127	0	119	0	0
2	f	127	0	119	0	0
2	g	127	0	119	0	0
2	h	127	0	119	0	0
3	A	25	0	0	1	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
3	H	10	0	0	0	0
3	a	5	0	0	0	0
3	b	5	0	0	0	0
3	c	5	0	0	0	0
3	d	5	0	0	0	0
3	f	5	0	0	0	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
All	All	11296	0	10778	49	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 4.

The worst 5 of 49 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:G:125:PRO:HD2	1:G:126:GLU:OE1	1.88	0.72
1:A:183:ARG:NH1	3:A:304:SO4:O1	2.27	0.68
1:B:70:SER:HB2	1:B:102:ILE:HD11	1.82	0.62
1:E:103:ARG:HH22	1:F:120:PRO:HG3	1.64	0.62
1:D:70:SER:HB2	1:D:102:ILE:HD11	1.85	0.58

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	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
1	B	159/205 (78%)	157 (99%)	2 (1%)	0	100	100
1	C	157/205 (77%)	156 (99%)	1 (1%)	0	100	100
1	D	158/205 (77%)	157 (99%)	1 (1%)	0	100	100
1	E	158/205 (77%)	158 (100%)	0	0	100	100
1	F	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
1	G	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
1	H	159/205 (78%)	157 (99%)	2 (1%)	0	100	100
2	a	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	b	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	c	12/14 (86%)	10 (83%)	2 (17%)	0	100	100
2	d	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	e	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	f	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	g	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	h	12/14 (86%)	10 (83%)	2 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1364/1752 (78%)	1345 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	136/171 (80%)	134 (98%)	2 (2%)	60	86
1	B	136/171 (80%)	135 (99%)	1 (1%)	81	94
1	C	135/171 (79%)	133 (98%)	2 (2%)	60	86
1	D	135/171 (79%)	133 (98%)	2 (2%)	60	86
1	E	135/171 (79%)	131 (97%)	4 (3%)	36	70
1	F	136/171 (80%)	134 (98%)	2 (2%)	60	86
1	G	136/171 (80%)	132 (97%)	4 (3%)	37	71
1	H	136/171 (80%)	134 (98%)	2 (2%)	60	86
2	a	13/13 (100%)	13 (100%)	0	100	100
2	b	13/13 (100%)	13 (100%)	0	100	100
2	c	13/13 (100%)	13 (100%)	0	100	100
2	d	13/13 (100%)	13 (100%)	0	100	100
2	e	13/13 (100%)	13 (100%)	0	100	100
2	f	13/13 (100%)	13 (100%)	0	100	100
2	g	13/13 (100%)	13 (100%)	0	100	100
2	h	13/13 (100%)	13 (100%)	0	100	100
All	All	1189/1472 (81%)	1170 (98%)	19 (2%)	58	85

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	142	ASN

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Mol	Chain	Res	Type
1	H	41	GLU
1	H	134	ARG
1	G	153	SER
1	E	89	ILE

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

28 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	$\# Z  > 2$
3	SO4	A	304	-	4,4,4	0.27	0	6,6,6	0.19	0
3	SO4	a	101	-	4,4,4	0.23	0	6,6,6	0.23	0
3	SO4	F	302	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	C	301	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	G	302	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	G	303	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	305	-	4,4,4	0.25	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	E	301	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	D	302	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	G	301	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	D	301	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	b	101	-	4,4,4	0.21	0	6,6,6	0.25	0
3	SO4	C	302	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	H	302	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	B	303	-	4,4,4	0.23	0	6,6,6	0.17	0
3	SO4	d	101	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	C	303	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	H	301	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	f	101	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.27	0
3	SO4	B	302	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	F	303	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	B	304	-	4,4,4	0.21	0	6,6,6	0.20	0
3	SO4	A	303	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.14	0
3	SO4	c	101	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	F	301	-	4,4,4	0.14	0	6,6,6	0.51	0
3	SO4	A	301	-	4,4,4	0.25	0	6,6,6	0.18	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	161/205 (78%)	0.07	3 (1%) 66 58	34, 48, 72, 81	0
1	B	161/205 (78%)	-0.06	3 (1%) 66 58	33, 47, 69, 88	0
1	C	159/205 (77%)	0.61	7 (4%) 39 32	41, 73, 104, 133	0
1	D	160/205 (78%)	0.17	2 (1%) 74 67	39, 59, 79, 92	0
1	E	160/205 (78%)	0.07	5 (3%) 51 43	34, 51, 72, 151	0
1	F	161/205 (78%)	-0.00	2 (1%) 76 69	31, 48, 70, 96	0
1	G	161/205 (78%)	0.57	10 (6%) 28 21	48, 68, 100, 128	0
1	H	161/205 (78%)	0.70	16 (9%) 14 11	49, 75, 108, 139	0
2	a	13/14 (92%)	0.15	1 (7%) 21 16	37, 39, 54, 65	0
2	b	13/14 (92%)	0.13	1 (7%) 21 16	35, 40, 53, 69	0
2	c	13/14 (92%)	1.61	4 (30%) 1 1	63, 71, 90, 94	0
2	d	13/14 (92%)	0.71	2 (15%) 6 5	46, 55, 65, 73	0
2	e	13/14 (92%)	0.46	1 (7%) 21 16	43, 50, 60, 71	0
2	f	13/14 (92%)	0.46	1 (7%) 21 16	39, 48, 65, 78	0
2	g	13/14 (92%)	0.60	1 (7%) 21 16	50, 57, 69, 82	0
2	h	13/14 (92%)	0.54	1 (7%) 21 16	53, 56, 61, 61	0
All	All	1388/1752 (79%)	0.29	60 (4%) 40 32	31, 58, 95, 151	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	196	LEU	5.6
1	H	40	ALA	4.5
1	A	196	LEU	4.5
1	F	196	LEU	4.3
1	G	196	LEU	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 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<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
3	SO4	C	303	5/5	0.72	0.18	94,97,101,115	0
3	SO4	F	303	5/5	0.74	0.24	73,79,84,101	0
3	SO4	b	101	5/5	0.76	0.20	76,83,90,90	0
3	SO4	E	301	5/5	0.77	0.17	67,76,87,90	0
3	SO4	G	302	5/5	0.78	0.14	83,89,98,100	0
3	SO4	F	302	5/5	0.79	0.17	68,76,94,97	0
3	SO4	A	302	5/5	0.80	0.18	71,79,92,97	0
3	SO4	A	303	5/5	0.80	0.17	57,69,92,92	0
3	SO4	H	301	5/5	0.80	0.12	89,93,99,102	0
3	SO4	A	305	5/5	0.80	0.17	78,78,92,94	0
3	SO4	C	302	5/5	0.82	0.13	85,91,97,100	0
3	SO4	B	303	5/5	0.82	0.19	71,71,97,100	0
3	SO4	B	304	5/5	0.83	0.21	71,72,79,83	0
3	SO4	B	302	5/5	0.84	0.13	71,74,86,87	0
3	SO4	G	303	5/5	0.85	0.16	85,86,101,112	0
3	SO4	G	301	5/5	0.85	0.15	76,77,89,90	0
3	SO4	C	301	5/5	0.85	0.15	75,76,86,97	0
3	SO4	a	101	5/5	0.86	0.16	73,74,88,90	0
3	SO4	D	302	5/5	0.86	0.17	73,82,89,94	0
3	SO4	c	101	5/5	0.88	0.10	75,86,87,90	0
3	SO4	d	101	5/5	0.89	0.17	63,65,67,67	0
3	SO4	A	304	5/5	0.90	0.21	76,77,92,94	0
3	SO4	f	101	5/5	0.90	0.17	63,64,73,76	0
3	SO4	H	302	5/5	0.91	0.14	71,73,85,88	0
3	SO4	B	301	5/5	0.92	0.15	52,58,67,76	0
3	SO4	D	301	5/5	0.93	0.14	51,52,62,63	0
3	SO4	A	301	5/5	0.95	0.08	59,66,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	F	301	5/5	0.96	0.07	26,39,42,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.