wwPDB X-ray Structure Validation Summary Report (i)

Feb 20, 2025 – 05:02 PM EST

PDB ID	:	9BT3
Title	:	Crystal structure of Chorismate Mutase from Mycobacterium tuberculosis in complex with the cyclic peptide inhibitor L2.1 (triclinic form)
Authors	:	Liu, L.; Lovell, S.; Battaile, K.P.; Inglese, J.
Deposited on	:	2024-05-14
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

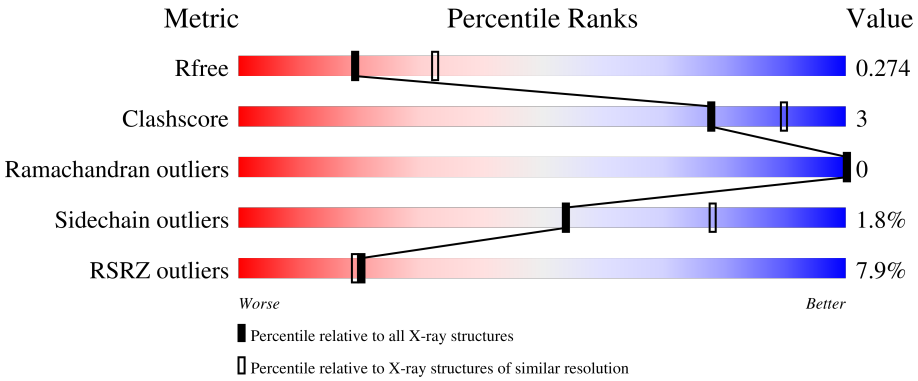
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	205	4% 73% 5% 21%
1	B	205	3% 73% 6% 21%
1	C	205	5% 74% 5% 21%
1	D	205	2% 77% • 21%
1	E	205	3% 76% • 21%

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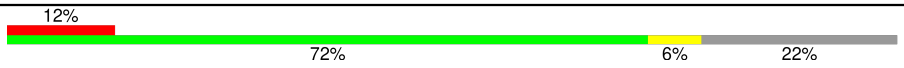
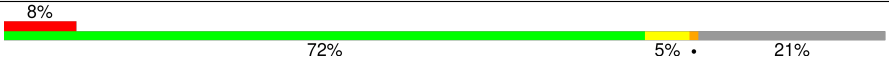
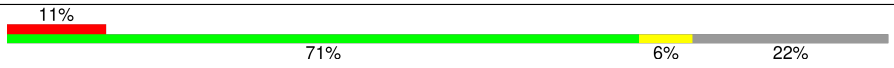
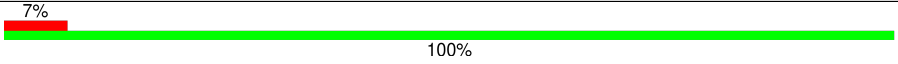
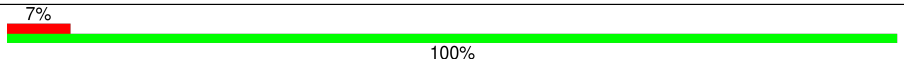
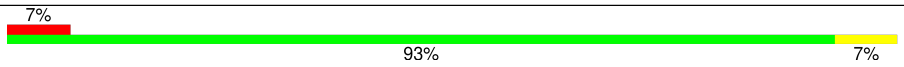
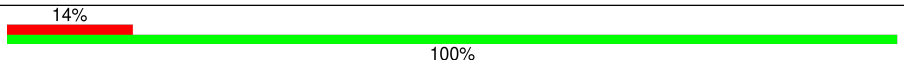
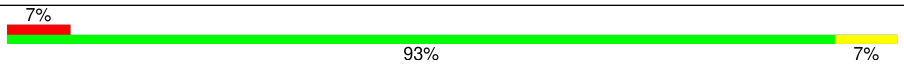
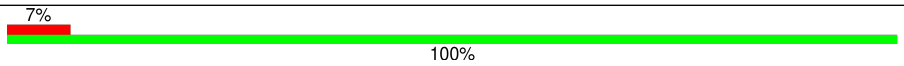
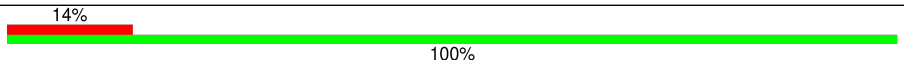
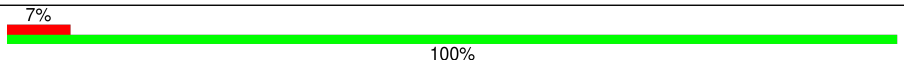
Mol	Chain	Length	Quality of chain
1	F	205	
1	G	205	
1	H	205	
2	a	14	
2	b	14	
2	c	14	
2	d	14	
2	e	14	
2	f	14	
2	g	14	
2	h	14	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11365 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	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	D	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	E	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	F	160	Total	C	N	O	S	0	0	0
			1262	781	230	248	3			
1	G	161	Total	C	N	O	S	0	0	0
			1270	787	231	249	3			
1	H	160	Total	C	N	O	S	0	0	0
			1262	781	230	248	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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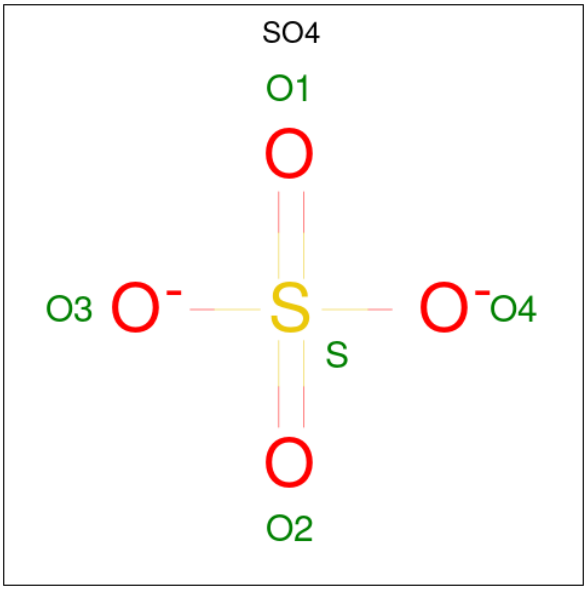
Chain	Residue	Modelled	Actual	Comment	Reference
H	234	HIS	-	expression tag	UNP P9WIB9
H	235	HIS	-	expression tag	UNP P9WIB9
H	236	HIS	-	expression tag	UNP P9WIB9
H	237	GLU	-	expression tag	UNP P9WIB9
H	238	LEU	-	expression tag	UNP P9WIB9

- 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_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	f	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

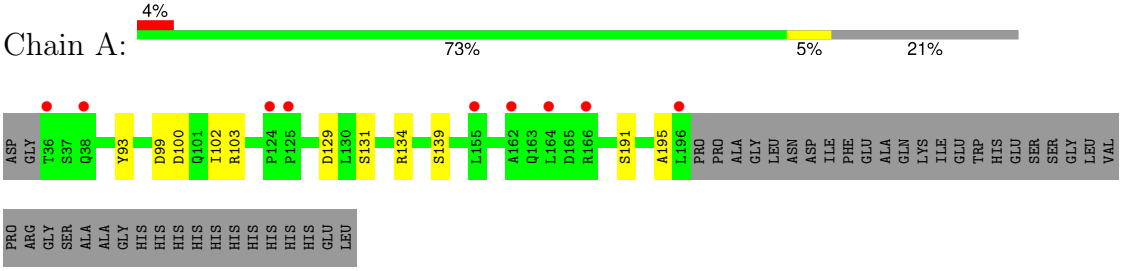
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	12	Total O 12 12	0	0
4	C	12	Total O 12 12	0	0
4	D	5	Total O 5 5	0	0
4	E	12	Total O 12 12	0	0
4	F	10	Total O 10 10	0	0
4	G	8	Total O 8 8	0	0
4	H	8	Total O 8 8	0	0
4	b	1	Total O 1 1	0	0
4	c	1	Total O 1 1	0	0
4	d	1	Total O 1 1	0	0
4	e	3	Total O 3 3	0	0
4	f	3	Total O 3 3	0	0
4	g	1	Total O 1 1	0	0
4	h	4	Total O 4 4	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.

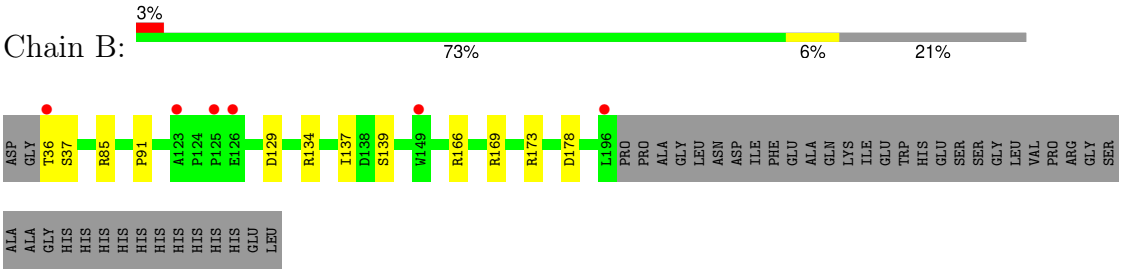
• Molecule 1: Secreted chorismate mutase

Chain A:



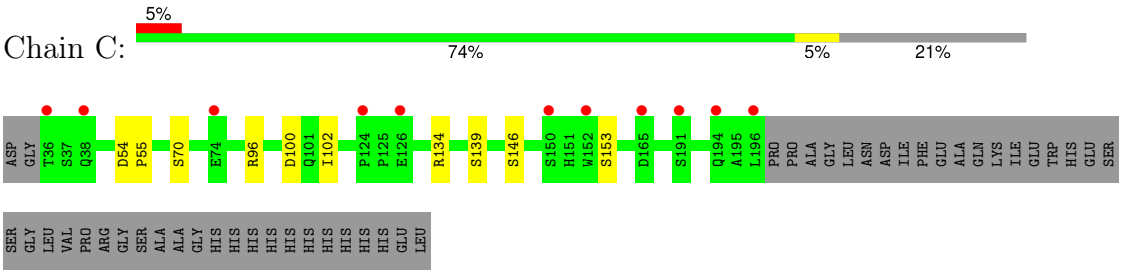
• Molecule 1: Secreted chorismate mutase

Chain B:



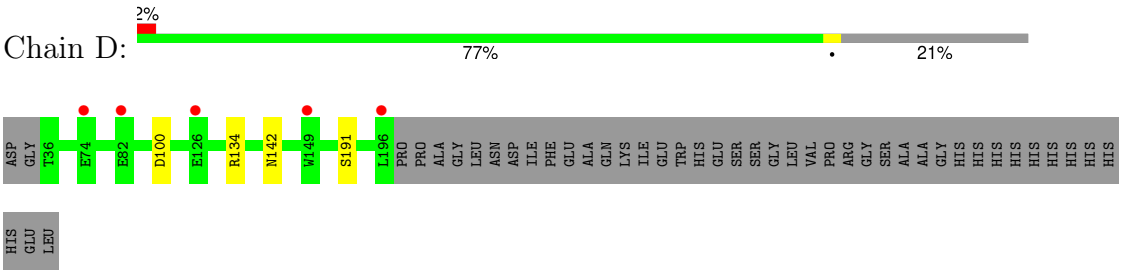
• Molecule 1: Secreted chorismate mutase

Chain C:



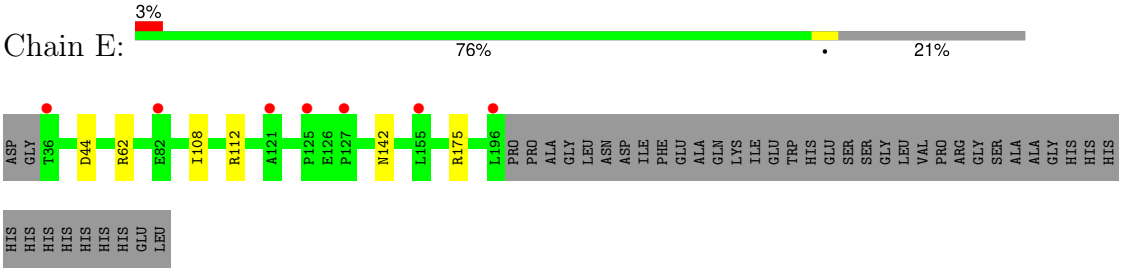
• Molecule 1: Secreted chorismate mutase

Chain D:



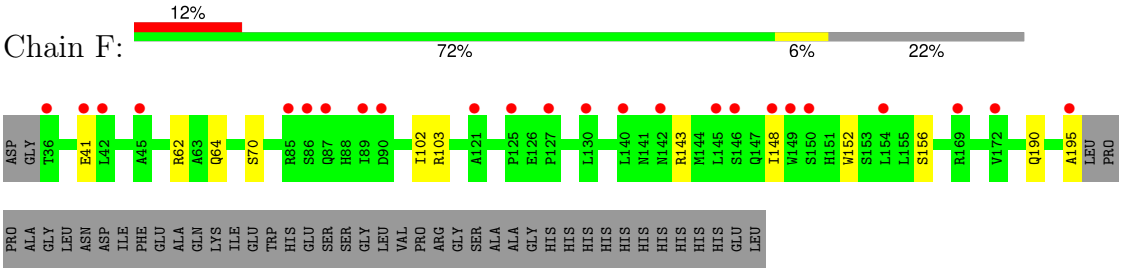
• Molecule 1: Secreted chorismate mutase

Chain E:



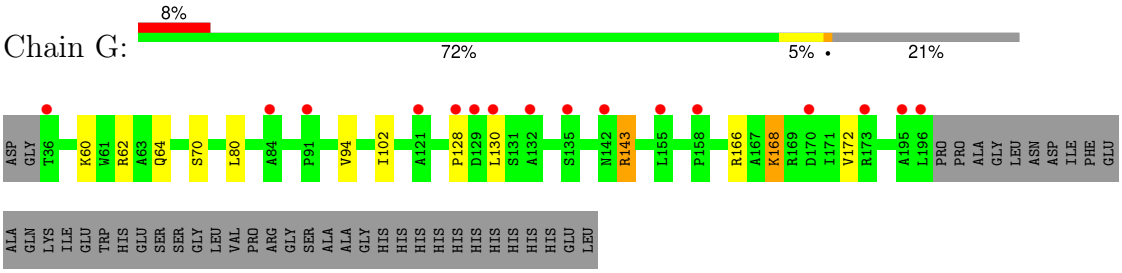
• Molecule 1: Secreted chorismate mutase

Chain F:



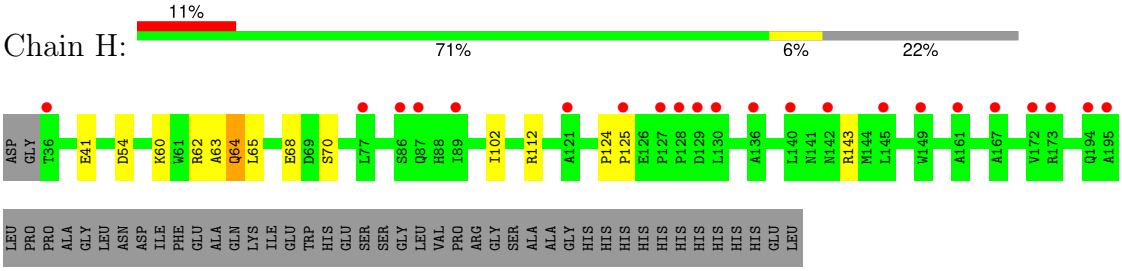
• Molecule 1: Secreted chorismate mutase

Chain G:



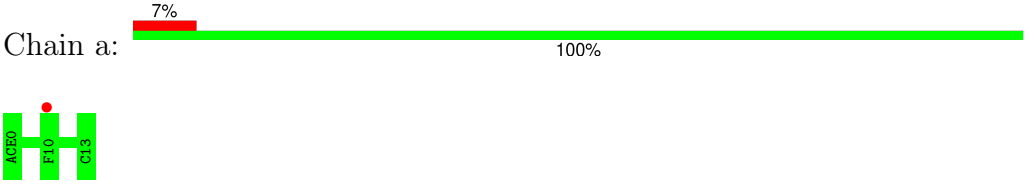
• Molecule 1: Secreted chorismate mutase

Chain H:



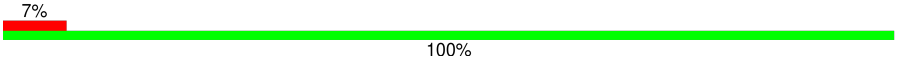
• Molecule 2: Peptide L2.1

Chain a:



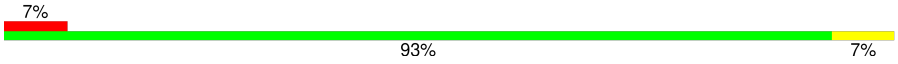
• Molecule 2: Peptide L2.1

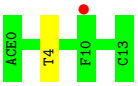
Chain b:



• Molecule 2: Peptide L2.1

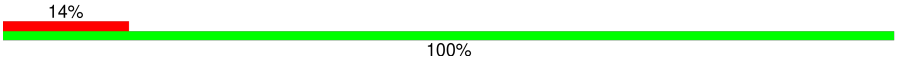
Chain c:





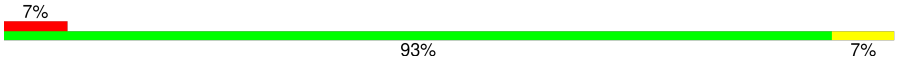
• Molecule 2: Peptide L2.1

Chain d:



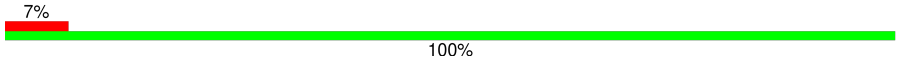
• Molecule 2: Peptide L2.1

Chain e:



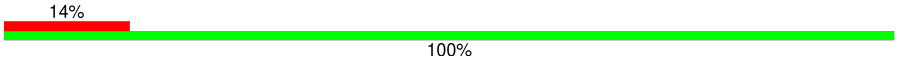
• Molecule 2: Peptide L2.1

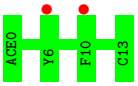
Chain f:



• Molecule 2: Peptide L2.1

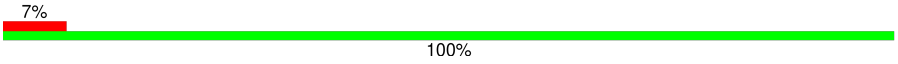
Chain g:





• Molecule 2: Peptide L2.1

Chain h:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.94Å 73.40Å 117.86Å 74.75° 82.21° 77.39°	Depositor
Resolution (Å)	38.72 – 2.50 38.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.72-2.50) 98.3 (38.72-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.229 , 0.275 0.231 , 0.274	Depositor DCC
R_{free} test set	3070 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.6	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	0.92	EDS
Total number of atoms	11365	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ACE, 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	0.49	0/1296	0.64	0/1764
1	B	0.54	0/1296	0.69	0/1764
1	C	0.54	0/1296	0.67	0/1764
1	D	0.51	0/1296	0.64	0/1764
1	E	0.52	0/1296	0.70	0/1764
1	F	0.47	0/1288	0.66	0/1753
1	G	0.47	0/1296	0.64	0/1764
1	H	0.45	0/1288	0.64	0/1753
2	a	0.72	0/131	0.65	0/178
2	b	0.68	0/131	0.80	0/178
2	c	0.78	0/131	0.70	0/178
2	d	0.81	0/131	0.84	0/178
2	e	0.89	1/131 (0.8%)	0.71	0/178
2	f	0.69	0/131	0.70	0/178
2	g	0.72	0/131	0.62	0/178
2	h	0.73	0/131	0.68	0/178
All	All	0.53	1/11400 (0.0%)	0.67	0/15514

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	13	CYS	CB-SG	-6.31	1.71	1.82

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	6	0
1	B	1270	0	1233	7	0
1	C	1270	0	1233	3	0
1	D	1270	0	1233	1	0
1	E	1270	0	1233	2	0
1	F	1262	0	1222	7	0
1	G	1270	0	1233	8	0
1	H	1262	0	1222	7	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	20	0	0	1	0
3	B	20	0	0	1	0
3	C	25	0	0	1	0
3	D	25	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	f	5	0	0	0	0
4	A	9	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	0	0
4	D	5	0	0	0	0
4	E	12	0	0	0	0
4	F	10	0	0	0	0
4	G	8	0	0	0	0
4	H	8	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
4	d	1	0	0	0	0
4	e	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	f	3	0	0	0	0
4	g	1	0	0	0	0
4	h	4	0	0	0	0
All	All	11365	0	10794	38	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 3.

The worst 5 of 38 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:143:ARG:HA	1:G:143:ARG:HE	1.52	0.74
1:D:100:ASP:OD2	1:D:191:SER:OG	2.07	0.73
1:F:103:ARG:NH2	1:F:190:GLN:OE1	2.23	0.72
1:F:156:SER:HA	1:F:195:ALA:HB3	1.76	0.68
1:F:152:TRP:CZ2	1:F:195:ALA:HB1	2.34	0.61

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	159/205 (78%)	157 (99%)	2 (1%)	0	100	100
1	D	159/205 (78%)	157 (99%)	2 (1%)	0	100	100
1	E	159/205 (78%)	155 (98%)	4 (2%)	0	100	100
1	F	158/205 (77%)	156 (99%)	2 (1%)	0	100	100
1	G	159/205 (78%)	156 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	158/205 (77%)	155 (98%)	3 (2%)	0	100	100
2	a	12/14 (86%)	10 (83%)	2 (17%)	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%)	11 (92%)	1 (8%)	0	100	100
All	All	1366/1752 (78%)	1337 (98%)	29 (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	136/171 (80%)	134 (98%)	2 (2%)	60	82
1	B	136/171 (80%)	132 (97%)	4 (3%)	37	64
1	C	136/171 (80%)	132 (97%)	4 (3%)	37	64
1	D	136/171 (80%)	134 (98%)	2 (2%)	60	82
1	E	136/171 (80%)	134 (98%)	2 (2%)	60	82
1	F	135/171 (79%)	134 (99%)	1 (1%)	81	93
1	G	136/171 (80%)	132 (97%)	4 (3%)	37	64
1	H	135/171 (79%)	133 (98%)	2 (2%)	60	82
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%)	12 (92%)	1 (8%)	10	22
2	d	13/13 (100%)	13 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	1190/1472 (81%)	1168 (98%)	22 (2%)	54	78

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	62	ARG
1	G	166	ARG
1	G	143	ARG
1	G	168	LYS
1	C	134	ARG

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)

23 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	H	301	-	4,4,4	0.29	0	6,6,6	0.22	0
3	SO4	D	301	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	f	101	-	4,4,4	0.44	0	6,6,6	0.22	0
3	SO4	B	302	-	4,4,4	0.31	0	6,6,6	0.12	0
3	SO4	G	301	-	4,4,4	0.30	0	6,6,6	0.62	0
3	SO4	C	305	-	4,4,4	0.37	0	6,6,6	0.30	0
3	SO4	C	301	-	4,4,4	0.26	0	6,6,6	0.50	0
3	SO4	B	304	-	4,4,4	0.35	0	6,6,6	0.46	0
3	SO4	B	303	-	4,4,4	0.33	0	6,6,6	0.40	0
3	SO4	A	302	-	4,4,4	0.32	0	6,6,6	0.46	0
3	SO4	C	302	-	4,4,4	0.37	0	6,6,6	0.44	0
3	SO4	E	301	-	4,4,4	0.29	0	6,6,6	0.86	0
3	SO4	A	304	-	4,4,4	0.29	0	6,6,6	0.21	0
3	SO4	F	301	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	D	303	-	4,4,4	0.29	0	6,6,6	0.32	0
3	SO4	B	301	-	4,4,4	0.28	0	6,6,6	0.47	0
3	SO4	C	304	-	4,4,4	0.27	0	6,6,6	0.20	0
3	SO4	D	302	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	A	303	-	4,4,4	0.27	0	6,6,6	0.35	0
3	SO4	C	303	-	4,4,4	0.33	0	6,6,6	0.18	0
3	SO4	D	304	-	4,4,4	0.39	0	6,6,6	0.30	0
3	SO4	D	305	-	4,4,4	0.37	0	6,6,6	0.36	0
3	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.50	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	SO4	1	0
3	A	304	SO4	1	0
3	C	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^{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	161/205 (78%)	0.61	9 (5%) 31 29	29, 46, 72, 88	0
1	B	161/205 (78%)	0.35	6 (3%) 45 42	26, 38, 55, 65	0
1	C	161/205 (78%)	0.51	11 (6%) 25 23	27, 38, 58, 74	0
1	D	161/205 (78%)	0.55	5 (3%) 51 48	29, 43, 66, 77	0
1	E	161/205 (78%)	0.54	7 (4%) 40 37	27, 42, 64, 83	0
1	F	160/205 (78%)	1.04	24 (15%) 6 6	26, 60, 86, 114	0
1	G	161/205 (78%)	0.89	16 (9%) 14 13	31, 58, 88, 109	0
1	H	160/205 (78%)	1.02	22 (13%) 8 7	31, 61, 91, 111	0
2	a	13/14 (92%)	0.60	1 (7%) 21 20	33, 38, 49, 57	0
2	b	13/14 (92%)	0.50	1 (7%) 21 20	28, 32, 42, 51	0
2	c	13/14 (92%)	0.63	1 (7%) 21 20	31, 33, 48, 48	0
2	d	13/14 (92%)	0.65	2 (15%) 6 6	30, 34, 53, 59	0
2	e	13/14 (92%)	0.58	1 (7%) 21 20	31, 38, 48, 54	0
2	f	13/14 (92%)	0.77	1 (7%) 21 20	39, 45, 57, 61	0
2	g	13/14 (92%)	1.22	2 (15%) 6 6	41, 50, 62, 64	0
2	h	13/14 (92%)	1.17	1 (7%) 21 20	42, 47, 61, 70	0
All	All	1390/1752 (79%)	0.69	110 (7%) 20 19	26, 45, 80, 114	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	196	LEU	6.4
1	H	121	ALA	5.2
1	F	89	ILE	5.2
1	G	196	LEU	4.7
2	h	10	PHE	4.6

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
3	SO4	A	302	5/5	0.73	0.18	67,70,71,90	0
3	SO4	B	304	5/5	0.75	0.17	57,62,67,84	0
3	SO4	C	305	5/5	0.75	0.21	62,63,72,85	0
3	SO4	D	305	5/5	0.75	0.19	64,65,69,86	0
3	SO4	A	304	5/5	0.76	0.21	72,74,86,87	0
3	SO4	A	303	5/5	0.78	0.24	67,67,70,73	0
3	SO4	C	302	5/5	0.80	0.17	63,70,83,87	0
3	SO4	H	301	5/5	0.81	0.13	67,71,94,95	0
3	SO4	D	303	5/5	0.82	0.15	67,68,88,93	0
3	SO4	f	101	5/5	0.82	0.15	51,62,69,74	0
3	SO4	F	301	5/5	0.83	0.16	65,68,79,81	0
3	SO4	B	303	5/5	0.84	0.18	55,62,79,87	0
3	SO4	C	303	5/5	0.86	0.20	58,59,62,68	0
3	SO4	D	304	5/5	0.89	0.14	53,58,70,71	0
3	SO4	C	304	5/5	0.90	0.14	64,71,75,78	0
3	SO4	A	301	5/5	0.92	0.11	46,49,61,76	0
3	SO4	D	302	5/5	0.92	0.13	63,63,71,72	0
3	SO4	B	301	5/5	0.92	0.15	50,55,59,63	0
3	SO4	C	301	5/5	0.92	0.15	56,61,69,71	0
3	SO4	D	301	5/5	0.93	0.12	50,54,63,64	0
3	SO4	B	302	5/5	0.93	0.15	44,59,67,68	0
3	SO4	G	301	5/5	0.94	0.13	33,34,41,47	0
3	SO4	E	301	5/5	0.96	0.08	28,31,37,72	0

6.5 Other polymers (i)

There are no such residues in this entry.