



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 19, 2019 – 11:59 AM EDT

PDB ID : 6AC6
Title : Ab initio crystal structure of Selenomethionine labelled Mycobacterium smegmatis Mfd
Authors : Putta, S.; Fox, G.C.; Walsh, M.A.; Rao, D.N.; Nagaraja, V.; Natesh, R.
Deposited on : 2018-07-25
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

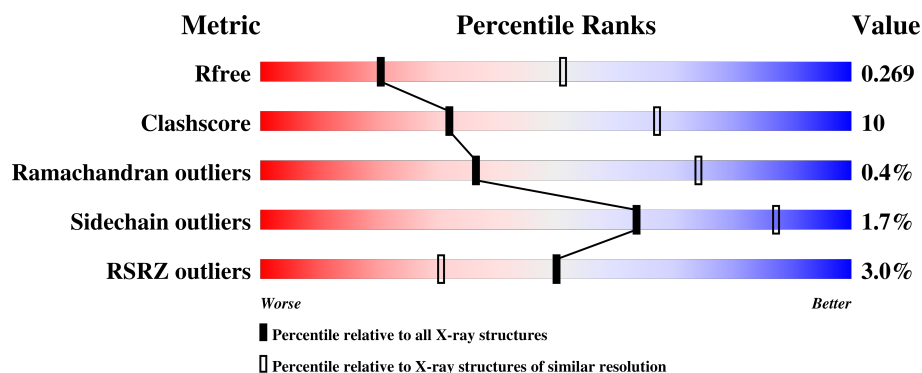
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	111664	2374 (3.00-2.96)
Clashscore	122126	2712 (3.00-2.96)
Ramachandran outliers	120053	2626 (3.00-2.96)
Sidechain outliers	120020	2629 (3.00-2.96)
RSRZ outliers	108989	2268 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1235	<div> <div>3%</div> <div>75%</div> <div>18%</div> <div>7%</div> </div>
1	B	1235	<div> <div>3%</div> <div>71%</div> <div>21%</div> <div>7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16853 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 Mycobacterium smegmatis Mfd.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1154	Total	C	N	O	S	Se	0	0	0
			8417	5293	1487	1606	6	25			
1	B	1153	Total	C	N	O	S	Se	0	0	0
			8337	5253	1473	1580	6	25			

There are 40 discrepancies between the modelled and reference sequences:

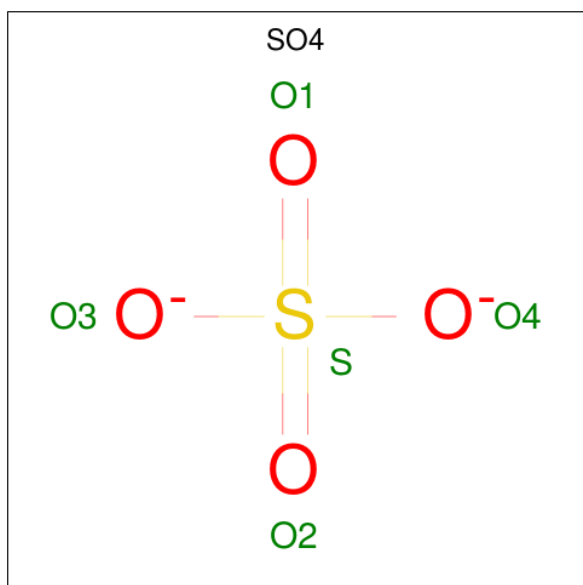
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	initiating methionine	UNP I7G7M2
A	-18	GLY	-	expression tag	UNP I7G7M2
A	-17	SER	-	expression tag	UNP I7G7M2
A	-16	SER	-	expression tag	UNP I7G7M2
A	-15	HIS	-	expression tag	UNP I7G7M2
A	-14	HIS	-	expression tag	UNP I7G7M2
A	-13	HIS	-	expression tag	UNP I7G7M2
A	-12	HIS	-	expression tag	UNP I7G7M2
A	-11	HIS	-	expression tag	UNP I7G7M2
A	-10	HIS	-	expression tag	UNP I7G7M2
A	-9	SER	-	expression tag	UNP I7G7M2
A	-8	SER	-	expression tag	UNP I7G7M2
A	-7	GLY	-	expression tag	UNP I7G7M2
A	-6	LEU	-	expression tag	UNP I7G7M2
A	-5	VAL	-	expression tag	UNP I7G7M2
A	-4	PRO	-	expression tag	UNP I7G7M2
A	-3	ARG	-	expression tag	UNP I7G7M2
A	-2	GLY	-	expression tag	UNP I7G7M2
A	-1	SER	-	expression tag	UNP I7G7M2
A	0	HIS	-	expression tag	UNP I7G7M2
B	-19	MSE	-	initiating methionine	UNP I7G7M2
B	-18	GLY	-	expression tag	UNP I7G7M2
B	-17	SER	-	expression tag	UNP I7G7M2
B	-16	SER	-	expression tag	UNP I7G7M2
B	-15	HIS	-	expression tag	UNP I7G7M2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP I7G7M2
B	-13	HIS	-	expression tag	UNP I7G7M2
B	-12	HIS	-	expression tag	UNP I7G7M2
B	-11	HIS	-	expression tag	UNP I7G7M2
B	-10	HIS	-	expression tag	UNP I7G7M2
B	-9	SER	-	expression tag	UNP I7G7M2
B	-8	SER	-	expression tag	UNP I7G7M2
B	-7	GLY	-	expression tag	UNP I7G7M2
B	-6	LEU	-	expression tag	UNP I7G7M2
B	-5	VAL	-	expression tag	UNP I7G7M2
B	-4	PRO	-	expression tag	UNP I7G7M2
B	-3	ARG	-	expression tag	UNP I7G7M2
B	-2	GLY	-	expression tag	UNP I7G7M2
B	-1	SER	-	expression tag	UNP I7G7M2
B	0	HIS	-	expression tag	UNP I7G7M2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

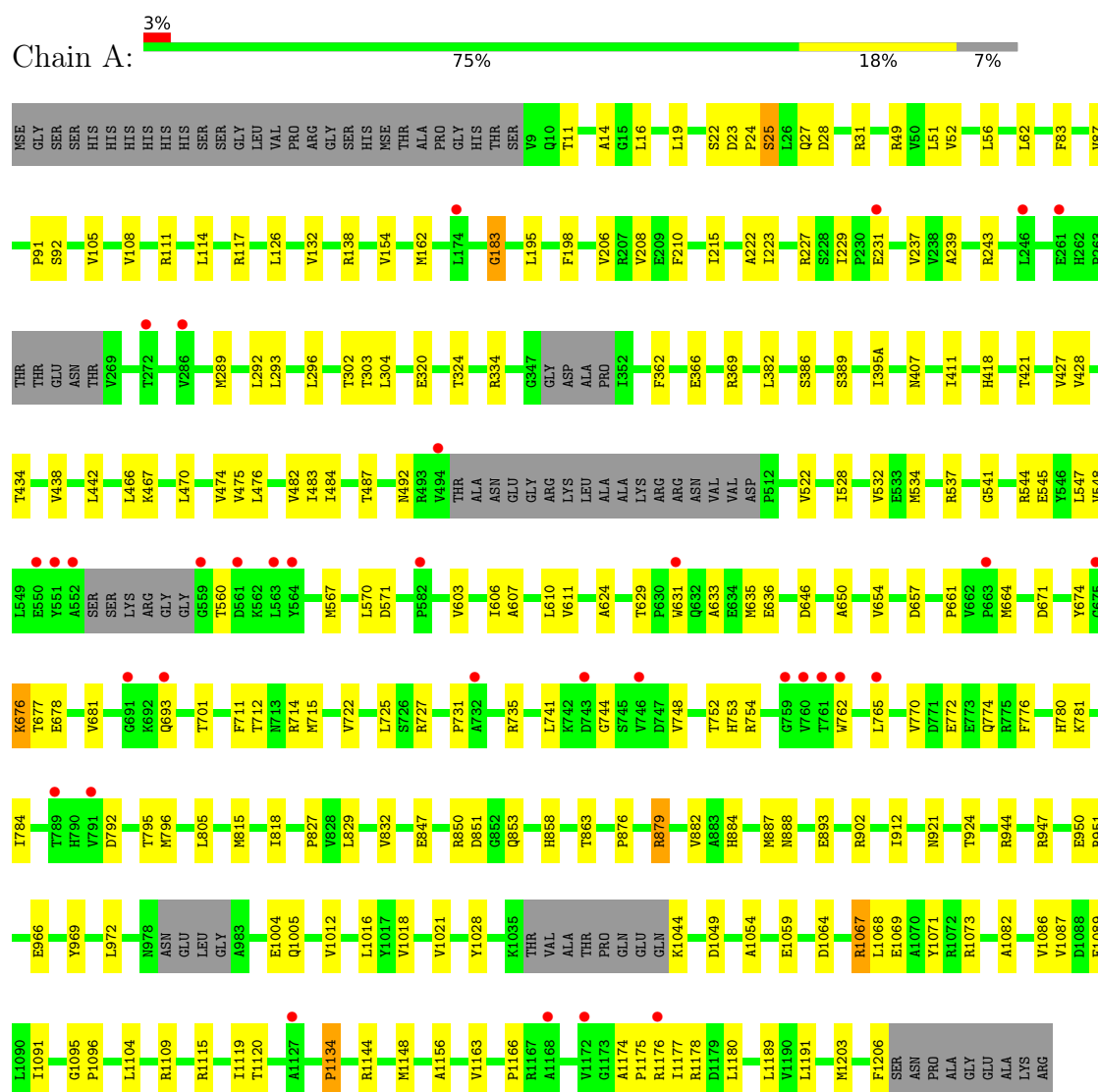
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	37	Total	O	0	0
			37	37		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Mycobacterium smegmatis Mfd



• Molecule 1: Mycobacterium smegmatis Mfd



L1193	T1036	T915	V793	G675	Q572	V474	S342	E209	L79	MSE
S1207	VAL	G916	L794	E678	L573	V475	G347	F210	R80	GLY
ASN	ALA	L917	T795	I679	A581	M480	G348	W211	F83	SER
PRO	THR	1926	S796	A680	L587	L481	D349	D212	S86	HIS
ALA	GLN	R929	S797	V681	G588	V482	A350	D213	V87	HIS
GLY	GLN	A930	P802	R682	G589	T483	P351	S216		HIS
GLU	GLN	D931	S808	Q693	S590	L484	L352	P90		HIS
ALA	GLN	L935	S808	Q693	S590	G491	L354	P91		HIS
LYS	ARG	S936	R813	T700	N594	M492	L354	S92		SER
ARG	V1052	Q937	E814	T701	T595	R227	R369	W93		SER
	S1063	L938	E814	L702	K596	S228	W379	E94		GLY
	D1064	H939	T817	L703	A599	A239	W380	L96		LEU
	E1069	Q940	E823	H707	R600	V240	T381	T95		VAL
	R1073	L941	E832	H710	V603	P241	S386	L96		PRO
	D1079	R944	V832	T714	V611	T248	V391	E99		ARG
	V1086	S948	D836	R714	Y614	T264	E392	R100		GLY
	E950	R949	Q839	G717	R617	THR	A401	P103		SER
	R951	V840	V840	F718	Q618	GLU	GLY	T107		ALA
	E1089	R846	R846	F719	Q618	LYS	ARG	R111		ALA
	Y1094	Q853	Q853	V720	A624	ARG	GLY	R120		GLY
	A1101	W722	W722	V721	A624	SER	GLY	THR		HIS
	V1105	K723	K723	W722	T629	GLN	GLY	VAL		THR
	C1114	S726	S726	W722	T629	GLN	GLY	T125		VAL
	I1119	R727	R727	W722	T629	GLN	GLY	T125		VAL
	T1129	R728	R728	W722	T629	GLN	GLY	T125		VAL
	S1133	L741	L741	W722	T629	GLN	GLY	T125		VAL
	P1134	K742	K742	W722	T629	GLN	GLY	T125		VAL
	R1144	D743	D743	W722	T629	GLN	GLY	T125		VAL
	L1145	V746	V746	W722	T629	GLN	GLY	T125		VAL
	R1155	G751	G751	W722	T629	GLN	GLY	T125		VAL
	T1158	L755	L755	W722	T629	GLN	GLY	T125		VAL
	P1164	L756	L756	W722	T629	GLN	GLY	T125		VAL
	V1172	L757	L757	W722	T629	GLN	GLY	T125		VAL
	GLY	L758	L758	W722	T629	GLN	GLY	T125		VAL
	A1174	L768	L768	W722	T629	GLN	GLY	T125		VAL
	I1177	L769	L769	W722	T629	GLN	GLY	T125		VAL
	R1178	L770	L770	W722	T629	GLN	GLY	T125		VAL
	D1179	L771	L771	W722	T629	GLN	GLY	T125		VAL
	L1182	L772	L772	W722	T629	GLN	GLY	T125		VAL
		L773	L773	W722	T629	GLN	GLY	T125		VAL
		L774	L774	W722	T629	GLN	GLY	T125		VAL
		L775	L775	W722	T629	GLN	GLY	T125		VAL
		L776	L776	W722	T629	GLN	GLY	T125		VAL
		L777	L777	W722	T629	GLN	GLY	T125		VAL
		L778	L778	W722	T629	GLN	GLY	T125		VAL
		L779	L779	W722	T629	GLN	GLY	T125		VAL
		L780	L780	W722	T629	GLN	GLY	T125		VAL
		L781	L781	W722	T629	GLN	GLY	T125		VAL
		L782	L782	W722	T629	GLN	GLY	T125		VAL
		L783	L783	W722	T629	GLN	GLY	T125		VAL
		L784	L784	W722	T629	GLN	GLY	T125		VAL
		L785	L785	W722	T629	GLN	GLY	T125		VAL
		L786	L786	W722	T629	GLN	GLY	T125		VAL
		L787	L787	W722	T629	GLN	GLY	T125		VAL
		L788	L788	W722	T629	GLN	GLY	T125		VAL
		L789	L789	W722	T629	GLN	GLY	T125		VAL
		L790	L790	W722	T629	GLN	GLY	T125		VAL
		L791	L791	W722	T629	GLN	GLY	T125		VAL
		L792	L792	W722	T629	GLN	GLY	T125		VAL
		L793	L793	W722	T629	GLN	GLY	T125		VAL
		L794	L794	W722	T629	GLN	GLY	T125		VAL
		L795	L795	W722	T629	GLN	GLY	T125		VAL
		L796	L796	W722	T629	GLN	GLY	T125		VAL
		L797	L797	W722	T629	GLN	GLY	T125		VAL
		L798	L798	W722	T629	GLN	GLY	T125		VAL
		L799	L799	W722	T629	GLN	GLY	T125		VAL
		L800	L800	W722	T629	GLN	GLY	T125		VAL
		L801	L801	W722	T629	GLN	GLY	T125		VAL
		L802	L802	W722	T629	GLN	GLY	T125		VAL
		L803	L803	W722	T629	GLN	GLY	T125		VAL
		L804	L804	W722	T629	GLN	GLY	T125		VAL
		L805	L805	W722	T629	GLN	GLY	T125		VAL
		L806	L806	W722	T629	GLN	GLY	T125		VAL
		L807	L807	W722	T629	GLN	GLY	T125		VAL
		L808	L808	W722	T629	GLN	GLY	T125		VAL
		L809	L809	W722	T629	GLN	GLY	T125		VAL
		L810	L810	W722	T629	GLN	GLY	T125		VAL
		L811	L811	W722	T629	GLN	GLY	T125		VAL
		L812	L812	W722	T629	GLN	GLY	T125		VAL
		L813	L813	W722	T629	GLN	GLY	T125		VAL
		L814	L814	W722	T629	GLN	GLY	T125		VAL
		L815	L815	W722	T629	GLN	GLY	T125		VAL
		L816	L816	W722	T629	GLN	GLY	T125		VAL
		L817	L817	W722	T629	GLN	GLY	T125		VAL
		L818	L818	W722	T629	GLN	GLY	T125		VAL
		L819	L819	W722	T629	GLN	GLY	T125		VAL
		L820	L820	W722	T629	GLN	GLY	T125		VAL
		L821	L821	W722	T629	GLN	GLY	T125		VAL
		L822	L822	W722	T629	GLN	GLY	T125		VAL
		L823	L823	W722	T629	GLN	GLY	T125		VAL
		L824	L824	W722	T629	GLN	GLY	T125		VAL
		L825	L825	W722	T629	GLN	GLY	T125		VAL
		L826	L826	W722	T629	GLN	GLY	T125		VAL
		L827	L827	W722	T629	GLN	GLY	T125		VAL
		L828	L828	W722	T629	GLN	GLY	T125		VAL
		L829	L829	W722	T629	GLN	GLY	T125		VAL
		L830	L830	W722	T629	GLN	GLY	T125		VAL
		L831	L831	W722	T629	GLN	GLY	T125		VAL
		L832	L832	W722	T629	GLN	GLY	T125		VAL
		L833	L833	W722	T629	GLN	GLY	T125		VAL
		L834	L834	W722	T629	GLN	GLY	T125		VAL
		L835	L835	W722	T629	GLN	GLY	T125		VAL
		L836	L836	W722	T629	GLN	GLY	T125		VAL
		L837	L837	W722	T629	GLN	GLY	T125		VAL
		L838	L838	W722	T629	GLN	GLY	T125		VAL
		L839	L839	W722	T629	GLN	GLY	T125		VAL
		L840	L840	W722	T629	GLN	GLY	T125		VAL
		L841	L841	W722	T629	GLN	GLY	T125		VAL
		L842	L842	W722	T629	GLN	GLY	T125		VAL
		L843	L843	W722	T629	GLN	GLY	T125		VAL
		L844	L844	W722	T629	GLN	GLY	T125		VAL
		L845	L845	W722	T629	GLN	GLY	T125		VAL
		L846	L846	W722	T629	GLN	GLY	T125		VAL
		L847	L847	W722	T629	GLN	GLY	T125		VAL
		L848	L848	W722	T629	GLN	GLY	T125		VAL
		L849	L849	W722	T629	GLN	GLY	T125		VAL
		L850	L850	W722	T629	GLN	GLY	T125		VAL
		L851	L851	W722	T629	GLN	GLY	T125		VAL
		L852	L852	W722	T629	GLN	GLY	T125		VAL
		L853	L853	W722	T629	GLN	GLY	T125		VAL
		L854	L854	W722	T629	GLN	GLY	T125		VAL
		L855	L855	W722	T629	GLN	GLY	T125		VAL
		L856	L856	W722	T629	GLN	GLY	T125		VAL
		L857	L857	W722	T629	GLN	GLY	T125		VAL
		L858	L858	W722	T629	GLN	GLY	T125		VAL
		L859	L859	W722	T629	GLN	GLY	T125		VAL
		L860	L860	W722	T629	GLN	GLY	T125		VAL
		L861	L861	W722	T629	GLN	GLY	T125		VAL
		L862	L862	W722	T629	GLN	GLY	T125		VAL
		L863	L863	W722	T629	GLN	GLY	T125		VAL
		L864	L864	W722	T629	GLN	GLY	T125		VAL
		L865	L865	W722	T629	GLN	GLY	T125		VAL
		L866	L866	W722	T629	GLN	GLY	T125		VAL
		L867	L867	W722	T629	GLN	GLY	T125		VAL
		L868	L868	W722	T629	GLN	GLY	T125		VAL
		L869	L869	W722	T629	GLN	GLY	T125		VAL
		L870	L870	W722	T629	GLN	GLY	T125		VAL
		L871	L871	W722	T629	GLN	GLY	T125		VAL
		L872	L872	W722	T629	GLN	GLY	T125		VAL
		L873	L873	W722	T629	GLN	GLY	T125		VAL
		L874	L874	W722	T629	GLN	GLY	T125		VAL
		L875	L875	W722	T629	GLN	GLY	T125		VAL
		L876	L876	W722	T629	GLN	GLY	T125		VAL
		L877	L877	W722	T629	GLN	GLY	T125		VAL
		L878	L878	W722	T629	GLN	GLY	T125		VAL
		L879	L879	W722	T629	GLN	GLY	T125		VAL
		L880	L880	W722	T629	GLN	GLY	T125		VAL
		L881	L881	W722	T629	GLN	GLY	T125		VAL
		L882	L882	W722	T629	GLN	GLY	T125		VAL
		L883	L883	W722	T629	GLN	GLY	T125		VAL
		L884	L884	W722	T629	GLN	GLY	T125		VAL
		L885	L885	W722	T629	GLN	GLY	T125		VAL

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.71Å 158.87Å 207.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.99 47.19 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.19-2.99) 96.5 (47.19-2.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.218 , 0.270 0.219 , 0.269	Depositor DCC
R_{free} test set	2788 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16853	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/8542	0.44	0/11635
1	B	0.27	0/8461	0.45	2/11529 (0.0%)
All	All	0.26	0/17003	0.45	2/23164 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	80	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	8417	0	8131	145	0
1	B	8337	0	8022	174	0
2	A	15	0	0	2	0
2	B	10	0	0	0	0
3	A	37	0	0	2	0
3	B	37	0	0	2	0
All	All	16853	0	16153	316	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 10.

The worst 5 of 316 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:B:452:LEU:HD13	1:B:466:LEU:HG	1.43	0.95
1:B:330:ILE:HD12	1:B:331:LYS:N	1.91	0.86
1:A:674:TYR:HB3	1:A:818:ILE:HD11	1.62	0.81
1:B:636:GLU:HG2	1:B:682:ARG:HH11	1.48	0.79
1:B:532:VAL:HG23	1:B:533:GLU:HB3	1.64	0.77

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	1140/1235 (92%)	1081 (95%)	56 (5%)	3 (0%)	43	78
1	B	1137/1235 (92%)	1070 (94%)	61 (5%)	6 (0%)	31	70
All	All	2277/2470 (92%)	2151 (94%)	117 (5%)	9 (0%)	36	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1134	PRO
1	B	588	GLY
1	A	560	THR
1	A	1134	PRO
1	B	248	THR

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	827/961 (86%)	809 (98%)	18 (2%)	55	83
1	B	807/961 (84%)	798 (99%)	9 (1%)	76	92
All	All	1634/1922 (85%)	1607 (98%)	27 (2%)	63	87

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	888	ASN
1	A	1176	ARG
1	B	860	ARG
1	A	1067	ARG
1	A	334	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	A	1301	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	A	1302	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	A	1303	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	B	1301	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	1302	-	4,4,4	0.16	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1129/1235 (91%)	0.11	34 (3%)	50	30	43, 76, 115, 138	0
1	B	1128/1235 (91%)	0.10	33 (2%)	51	31	46, 82, 116, 153	0
All	All	2257/2470 (91%)	0.11	67 (2%)	50	30	43, 78, 115, 153	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	717	GLY	4.6
1	B	463	VAL	4.5
1	A	552	ALA	4.3
1	B	540	GLY	4.2
1	B	349	ASP	4.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	1302	5/5	0.81	0.16	121,128,130,135	0
2	SO4	A	1303	5/5	0.97	0.17	78,81,90,90	0
2	SO4	A	1302	5/5	0.97	0.18	63,63,64,64	0
2	SO4	B	1301	5/5	0.98	0.15	61,66,69,76	0
2	SO4	A	1301	5/5	0.98	0.13	63,69,78,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.