wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 09:59 PM EDT

PDB ID	:	6ZNK
Title	:	MaeB PTA domain N718D mutant
Authors	:	Lovering, A.L.; Harding, C.J.
Deposited on	:	2020-07-06
Resolution	:	3.04 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 (1)) were used in the production of this report:

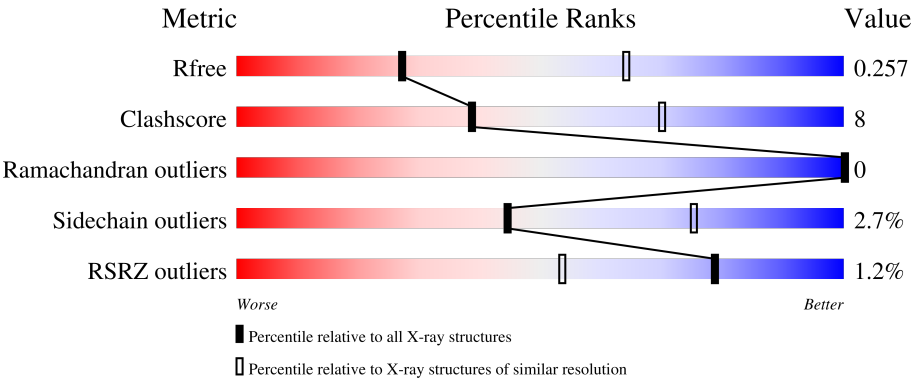
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.04 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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	362	73% 18% • 7%
1	B	362	% 79% 14% 7%
1	C	362	% 80% 14% 6%
1	D	362	% 72% 21% • 6%
1	E	362	2% 77% 15% • 7%

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Mol	Chain	Length	Quality of chain
1	F	362	79% 14% 7%
1	G	362	77% 15% 7%
1	H	362	75% 16% 7%
1	I	362	3% 79% 14% 7%
1	J	362	% 75% 18% 7%
1	K	362	4% 75% 18% 7%
1	L	362	% 75% 17% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	802	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31317 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	B	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	D	340	Total	C	N	O	S	0	0	0
			2614	1667	447	489	11			
1	F	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	E	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	C	339	Total	C	N	O	S	0	0	0
			2603	1661	444	487	11			
1	G	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	H	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	I	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	J	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	K	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			
1	L	338	Total	C	N	O	S	0	0	0
			2598	1658	443	486	11			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	initiating methionine	UNP Q6MM15
A	420	GLY	-	expression tag	UNP Q6MM15
A	421	SER	-	expression tag	UNP Q6MM15
A	422	SER	-	expression tag	UNP Q6MM15
A	423	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP Q6MM15
A	425	HIS	-	expression tag	UNP Q6MM15
A	426	HIS	-	expression tag	UNP Q6MM15
A	427	HIS	-	expression tag	UNP Q6MM15
A	428	HIS	-	expression tag	UNP Q6MM15
A	429	SER	-	expression tag	UNP Q6MM15
A	430	SER	-	expression tag	UNP Q6MM15
A	431	GLY	-	expression tag	UNP Q6MM15
A	432	LEU	-	expression tag	UNP Q6MM15
A	433	VAL	-	expression tag	UNP Q6MM15
A	434	PRO	-	expression tag	UNP Q6MM15
A	435	ALA	-	expression tag	UNP Q6MM15
A	436	GLY	-	expression tag	UNP Q6MM15
A	437	SER	-	expression tag	UNP Q6MM15
A	438	HIS	-	expression tag	UNP Q6MM15
A	718	ASP	ASN	engineered mutation	UNP Q6MM15
B	419	MET	-	initiating methionine	UNP Q6MM15
B	420	GLY	-	expression tag	UNP Q6MM15
B	421	SER	-	expression tag	UNP Q6MM15
B	422	SER	-	expression tag	UNP Q6MM15
B	423	HIS	-	expression tag	UNP Q6MM15
B	424	HIS	-	expression tag	UNP Q6MM15
B	425	HIS	-	expression tag	UNP Q6MM15
B	426	HIS	-	expression tag	UNP Q6MM15
B	427	HIS	-	expression tag	UNP Q6MM15
B	428	HIS	-	expression tag	UNP Q6MM15
B	429	SER	-	expression tag	UNP Q6MM15
B	430	SER	-	expression tag	UNP Q6MM15
B	431	GLY	-	expression tag	UNP Q6MM15
B	432	LEU	-	expression tag	UNP Q6MM15
B	433	VAL	-	expression tag	UNP Q6MM15
B	434	PRO	-	expression tag	UNP Q6MM15
B	435	ALA	-	expression tag	UNP Q6MM15
B	436	GLY	-	expression tag	UNP Q6MM15
B	437	SER	-	expression tag	UNP Q6MM15
B	438	HIS	-	expression tag	UNP Q6MM15
B	718	ASP	ASN	engineered mutation	UNP Q6MM15
D	419	MET	-	initiating methionine	UNP Q6MM15
D	420	GLY	-	expression tag	UNP Q6MM15
D	421	SER	-	expression tag	UNP Q6MM15
D	422	SER	-	expression tag	UNP Q6MM15
D	423	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
D	424	HIS	-	expression tag	UNP Q6MM15
D	425	HIS	-	expression tag	UNP Q6MM15
D	426	HIS	-	expression tag	UNP Q6MM15
D	427	HIS	-	expression tag	UNP Q6MM15
D	428	HIS	-	expression tag	UNP Q6MM15
D	429	SER	-	expression tag	UNP Q6MM15
D	430	SER	-	expression tag	UNP Q6MM15
D	431	GLY	-	expression tag	UNP Q6MM15
D	432	LEU	-	expression tag	UNP Q6MM15
D	433	VAL	-	expression tag	UNP Q6MM15
D	434	PRO	-	expression tag	UNP Q6MM15
D	435	ALA	-	expression tag	UNP Q6MM15
D	436	GLY	-	expression tag	UNP Q6MM15
D	437	SER	-	expression tag	UNP Q6MM15
D	438	HIS	-	expression tag	UNP Q6MM15
D	718	ASP	ASN	engineered mutation	UNP Q6MM15
F	419	MET	-	initiating methionine	UNP Q6MM15
F	420	GLY	-	expression tag	UNP Q6MM15
F	421	SER	-	expression tag	UNP Q6MM15
F	422	SER	-	expression tag	UNP Q6MM15
F	423	HIS	-	expression tag	UNP Q6MM15
F	424	HIS	-	expression tag	UNP Q6MM15
F	425	HIS	-	expression tag	UNP Q6MM15
F	426	HIS	-	expression tag	UNP Q6MM15
F	427	HIS	-	expression tag	UNP Q6MM15
F	428	HIS	-	expression tag	UNP Q6MM15
F	429	SER	-	expression tag	UNP Q6MM15
F	430	SER	-	expression tag	UNP Q6MM15
F	431	GLY	-	expression tag	UNP Q6MM15
F	432	LEU	-	expression tag	UNP Q6MM15
F	433	VAL	-	expression tag	UNP Q6MM15
F	434	PRO	-	expression tag	UNP Q6MM15
F	435	ALA	-	expression tag	UNP Q6MM15
F	436	GLY	-	expression tag	UNP Q6MM15
F	437	SER	-	expression tag	UNP Q6MM15
F	438	HIS	-	expression tag	UNP Q6MM15
F	718	ASP	ASN	engineered mutation	UNP Q6MM15
E	419	MET	-	initiating methionine	UNP Q6MM15
E	420	GLY	-	expression tag	UNP Q6MM15
E	421	SER	-	expression tag	UNP Q6MM15
E	422	SER	-	expression tag	UNP Q6MM15
E	423	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
E	424	HIS	-	expression tag	UNP Q6MM15
E	425	HIS	-	expression tag	UNP Q6MM15
E	426	HIS	-	expression tag	UNP Q6MM15
E	427	HIS	-	expression tag	UNP Q6MM15
E	428	HIS	-	expression tag	UNP Q6MM15
E	429	SER	-	expression tag	UNP Q6MM15
E	430	SER	-	expression tag	UNP Q6MM15
E	431	GLY	-	expression tag	UNP Q6MM15
E	432	LEU	-	expression tag	UNP Q6MM15
E	433	VAL	-	expression tag	UNP Q6MM15
E	434	PRO	-	expression tag	UNP Q6MM15
E	435	ALA	-	expression tag	UNP Q6MM15
E	436	GLY	-	expression tag	UNP Q6MM15
E	437	SER	-	expression tag	UNP Q6MM15
E	438	HIS	-	expression tag	UNP Q6MM15
E	718	ASP	ASN	engineered mutation	UNP Q6MM15
C	419	MET	-	initiating methionine	UNP Q6MM15
C	420	GLY	-	expression tag	UNP Q6MM15
C	421	SER	-	expression tag	UNP Q6MM15
C	422	SER	-	expression tag	UNP Q6MM15
C	423	HIS	-	expression tag	UNP Q6MM15
C	424	HIS	-	expression tag	UNP Q6MM15
C	425	HIS	-	expression tag	UNP Q6MM15
C	426	HIS	-	expression tag	UNP Q6MM15
C	427	HIS	-	expression tag	UNP Q6MM15
C	428	HIS	-	expression tag	UNP Q6MM15
C	429	SER	-	expression tag	UNP Q6MM15
C	430	SER	-	expression tag	UNP Q6MM15
C	431	GLY	-	expression tag	UNP Q6MM15
C	432	LEU	-	expression tag	UNP Q6MM15
C	433	VAL	-	expression tag	UNP Q6MM15
C	434	PRO	-	expression tag	UNP Q6MM15
C	435	ALA	-	expression tag	UNP Q6MM15
C	436	GLY	-	expression tag	UNP Q6MM15
C	437	SER	-	expression tag	UNP Q6MM15
C	438	HIS	-	expression tag	UNP Q6MM15
C	718	ASP	ASN	engineered mutation	UNP Q6MM15
G	419	MET	-	initiating methionine	UNP Q6MM15
G	420	GLY	-	expression tag	UNP Q6MM15
G	421	SER	-	expression tag	UNP Q6MM15
G	422	SER	-	expression tag	UNP Q6MM15
G	423	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
G	424	HIS	-	expression tag	UNP Q6MM15
G	425	HIS	-	expression tag	UNP Q6MM15
G	426	HIS	-	expression tag	UNP Q6MM15
G	427	HIS	-	expression tag	UNP Q6MM15
G	428	HIS	-	expression tag	UNP Q6MM15
G	429	SER	-	expression tag	UNP Q6MM15
G	430	SER	-	expression tag	UNP Q6MM15
G	431	GLY	-	expression tag	UNP Q6MM15
G	432	LEU	-	expression tag	UNP Q6MM15
G	433	VAL	-	expression tag	UNP Q6MM15
G	434	PRO	-	expression tag	UNP Q6MM15
G	435	ALA	-	expression tag	UNP Q6MM15
G	436	GLY	-	expression tag	UNP Q6MM15
G	437	SER	-	expression tag	UNP Q6MM15
G	438	HIS	-	expression tag	UNP Q6MM15
G	718	ASP	ASN	engineered mutation	UNP Q6MM15
H	419	MET	-	initiating methionine	UNP Q6MM15
H	420	GLY	-	expression tag	UNP Q6MM15
H	421	SER	-	expression tag	UNP Q6MM15
H	422	SER	-	expression tag	UNP Q6MM15
H	423	HIS	-	expression tag	UNP Q6MM15
H	424	HIS	-	expression tag	UNP Q6MM15
H	425	HIS	-	expression tag	UNP Q6MM15
H	426	HIS	-	expression tag	UNP Q6MM15
H	427	HIS	-	expression tag	UNP Q6MM15
H	428	HIS	-	expression tag	UNP Q6MM15
H	429	SER	-	expression tag	UNP Q6MM15
H	430	SER	-	expression tag	UNP Q6MM15
H	431	GLY	-	expression tag	UNP Q6MM15
H	432	LEU	-	expression tag	UNP Q6MM15
H	433	VAL	-	expression tag	UNP Q6MM15
H	434	PRO	-	expression tag	UNP Q6MM15
H	435	ALA	-	expression tag	UNP Q6MM15
H	436	GLY	-	expression tag	UNP Q6MM15
H	437	SER	-	expression tag	UNP Q6MM15
H	438	HIS	-	expression tag	UNP Q6MM15
H	718	ASP	ASN	engineered mutation	UNP Q6MM15
I	419	MET	-	initiating methionine	UNP Q6MM15
I	420	GLY	-	expression tag	UNP Q6MM15
I	421	SER	-	expression tag	UNP Q6MM15
I	422	SER	-	expression tag	UNP Q6MM15
I	423	HIS	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
I	424	HIS	-	expression tag	UNP Q6MM15
I	425	HIS	-	expression tag	UNP Q6MM15
I	426	HIS	-	expression tag	UNP Q6MM15
I	427	HIS	-	expression tag	UNP Q6MM15
I	428	HIS	-	expression tag	UNP Q6MM15
I	429	SER	-	expression tag	UNP Q6MM15
I	430	SER	-	expression tag	UNP Q6MM15
I	431	GLY	-	expression tag	UNP Q6MM15
I	432	LEU	-	expression tag	UNP Q6MM15
I	433	VAL	-	expression tag	UNP Q6MM15
I	434	PRO	-	expression tag	UNP Q6MM15
I	435	ALA	-	expression tag	UNP Q6MM15
I	436	GLY	-	expression tag	UNP Q6MM15
I	437	SER	-	expression tag	UNP Q6MM15
I	438	HIS	-	expression tag	UNP Q6MM15
I	718	ASP	ASN	engineered mutation	UNP Q6MM15
J	419	MET	-	initiating methionine	UNP Q6MM15
J	420	GLY	-	expression tag	UNP Q6MM15
J	421	SER	-	expression tag	UNP Q6MM15
J	422	SER	-	expression tag	UNP Q6MM15
J	423	HIS	-	expression tag	UNP Q6MM15
J	424	HIS	-	expression tag	UNP Q6MM15
J	425	HIS	-	expression tag	UNP Q6MM15
J	426	HIS	-	expression tag	UNP Q6MM15
J	427	HIS	-	expression tag	UNP Q6MM15
J	428	HIS	-	expression tag	UNP Q6MM15
J	429	SER	-	expression tag	UNP Q6MM15
J	430	SER	-	expression tag	UNP Q6MM15
J	431	GLY	-	expression tag	UNP Q6MM15
J	432	LEU	-	expression tag	UNP Q6MM15
J	433	VAL	-	expression tag	UNP Q6MM15
J	434	PRO	-	expression tag	UNP Q6MM15
J	435	ALA	-	expression tag	UNP Q6MM15
J	436	GLY	-	expression tag	UNP Q6MM15
J	437	SER	-	expression tag	UNP Q6MM15
J	438	HIS	-	expression tag	UNP Q6MM15
J	718	ASP	ASN	engineered mutation	UNP Q6MM15
K	419	MET	-	initiating methionine	UNP Q6MM15
K	420	GLY	-	expression tag	UNP Q6MM15
K	421	SER	-	expression tag	UNP Q6MM15
K	422	SER	-	expression tag	UNP Q6MM15
K	423	HIS	-	expression tag	UNP Q6MM15

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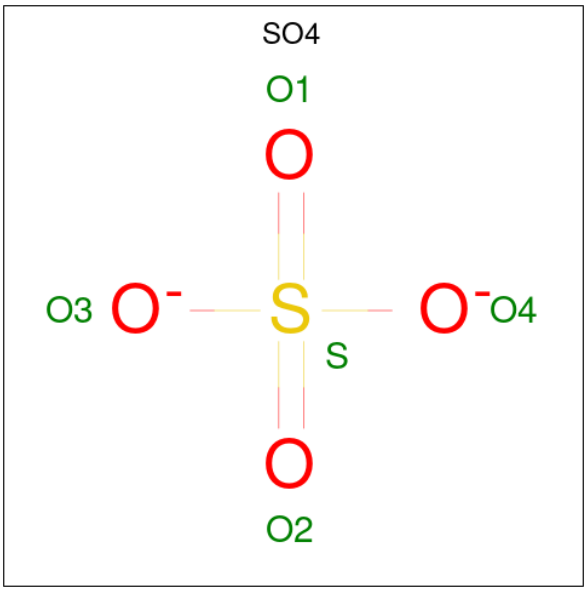
Chain	Residue	Modelled	Actual	Comment	Reference
K	424	HIS	-	expression tag	UNP Q6MM15
K	425	HIS	-	expression tag	UNP Q6MM15
K	426	HIS	-	expression tag	UNP Q6MM15
K	427	HIS	-	expression tag	UNP Q6MM15
K	428	HIS	-	expression tag	UNP Q6MM15
K	429	SER	-	expression tag	UNP Q6MM15
K	430	SER	-	expression tag	UNP Q6MM15
K	431	GLY	-	expression tag	UNP Q6MM15
K	432	LEU	-	expression tag	UNP Q6MM15
K	433	VAL	-	expression tag	UNP Q6MM15
K	434	PRO	-	expression tag	UNP Q6MM15
K	435	ALA	-	expression tag	UNP Q6MM15
K	436	GLY	-	expression tag	UNP Q6MM15
K	437	SER	-	expression tag	UNP Q6MM15
K	438	HIS	-	expression tag	UNP Q6MM15
K	718	ASP	ASN	engineered mutation	UNP Q6MM15
L	419	MET	-	initiating methionine	UNP Q6MM15
L	420	GLY	-	expression tag	UNP Q6MM15
L	421	SER	-	expression tag	UNP Q6MM15
L	422	SER	-	expression tag	UNP Q6MM15
L	423	HIS	-	expression tag	UNP Q6MM15
L	424	HIS	-	expression tag	UNP Q6MM15
L	425	HIS	-	expression tag	UNP Q6MM15
L	426	HIS	-	expression tag	UNP Q6MM15
L	427	HIS	-	expression tag	UNP Q6MM15
L	428	HIS	-	expression tag	UNP Q6MM15
L	429	SER	-	expression tag	UNP Q6MM15
L	430	SER	-	expression tag	UNP Q6MM15
L	431	GLY	-	expression tag	UNP Q6MM15
L	432	LEU	-	expression tag	UNP Q6MM15
L	433	VAL	-	expression tag	UNP Q6MM15
L	434	PRO	-	expression tag	UNP Q6MM15
L	435	ALA	-	expression tag	UNP Q6MM15
L	436	GLY	-	expression tag	UNP Q6MM15
L	437	SER	-	expression tag	UNP Q6MM15
L	438	HIS	-	expression tag	UNP Q6MM15
L	718	ASP	ASN	engineered mutation	UNP Q6MM15

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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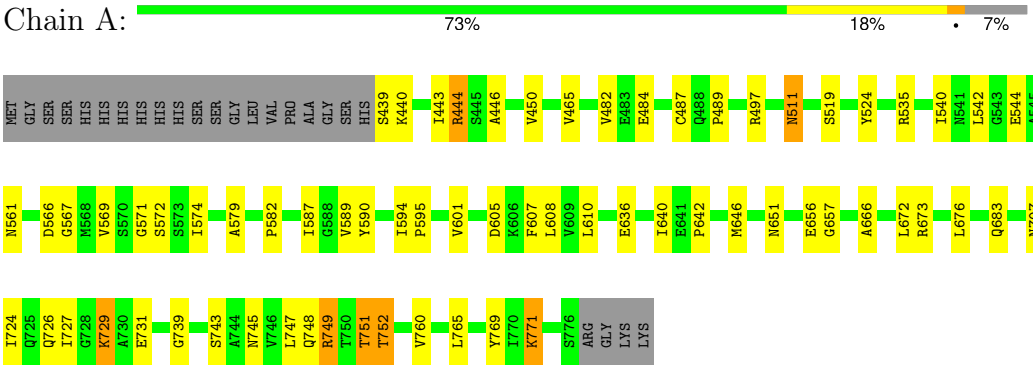
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

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.

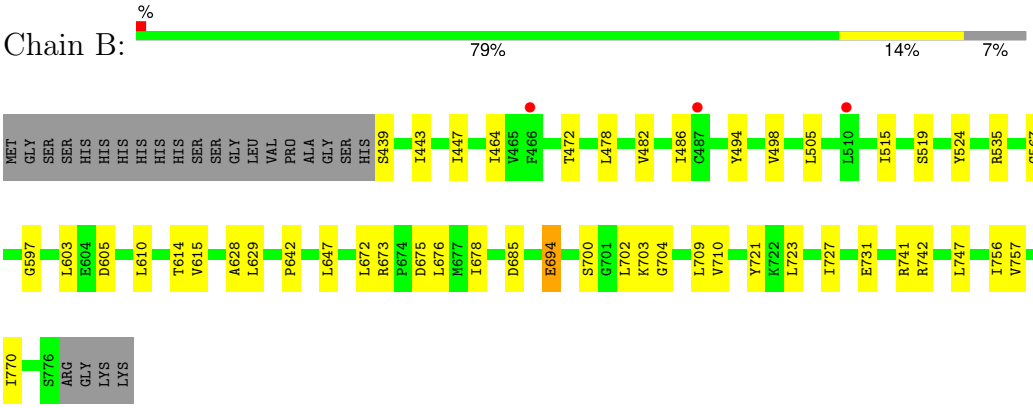
• Molecule 1: Malate dehydrogenase

Chain A:



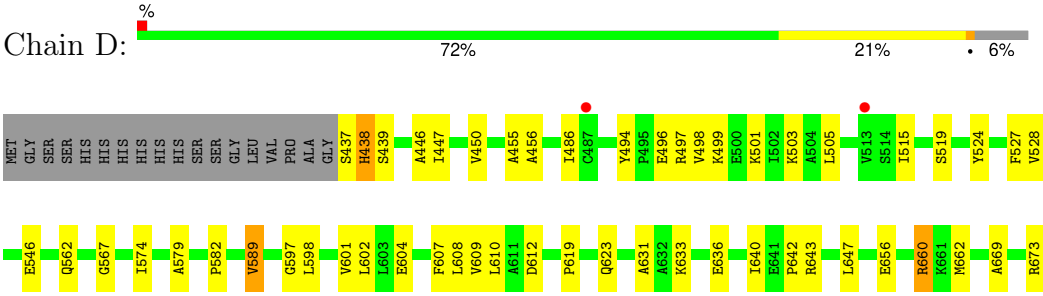
• Molecule 1: Malate dehydrogenase

Chain B:



• Molecule 1: Malate dehydrogenase

Chain D:

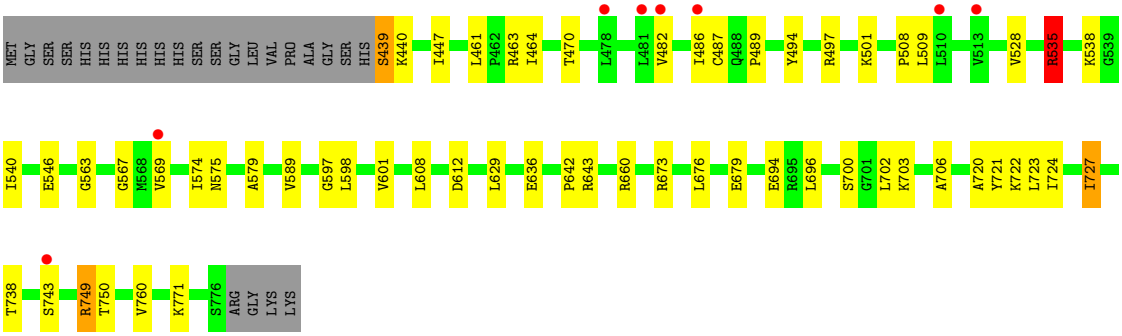


• Molecule 1: Malate dehydrogenase

Chain F:

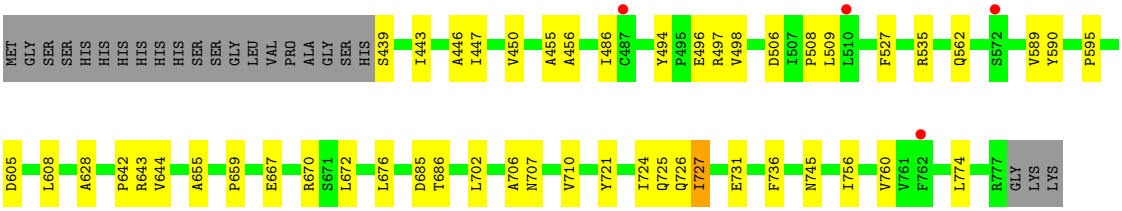
• Molecule 1: Malate dehydrogenase

Chain E:



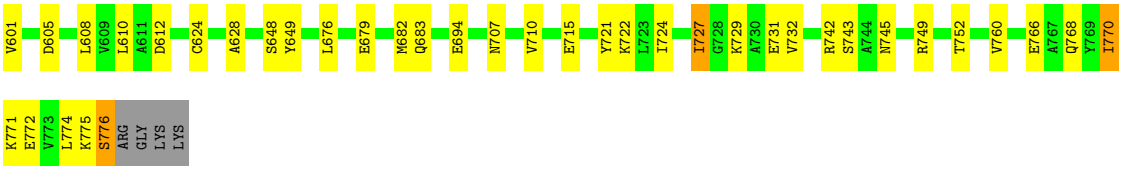
• Molecule 1: Malate dehydrogenase

Chain C:



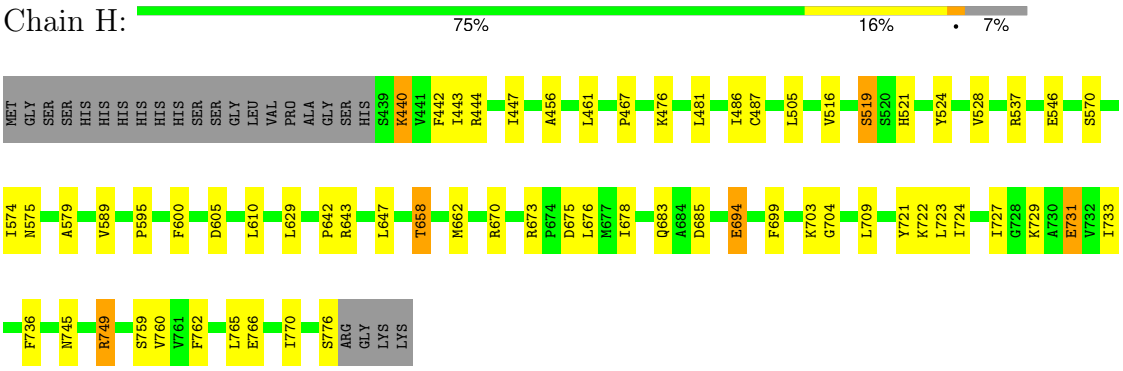
• Molecule 1: Malate dehydrogenase

Chain G:



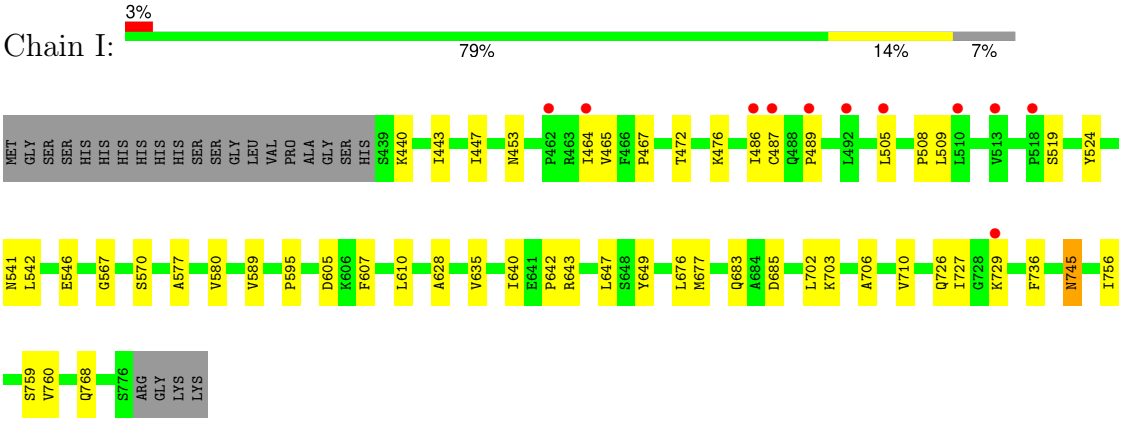
• Molecule 1: Malate dehydrogenase

Chain H:



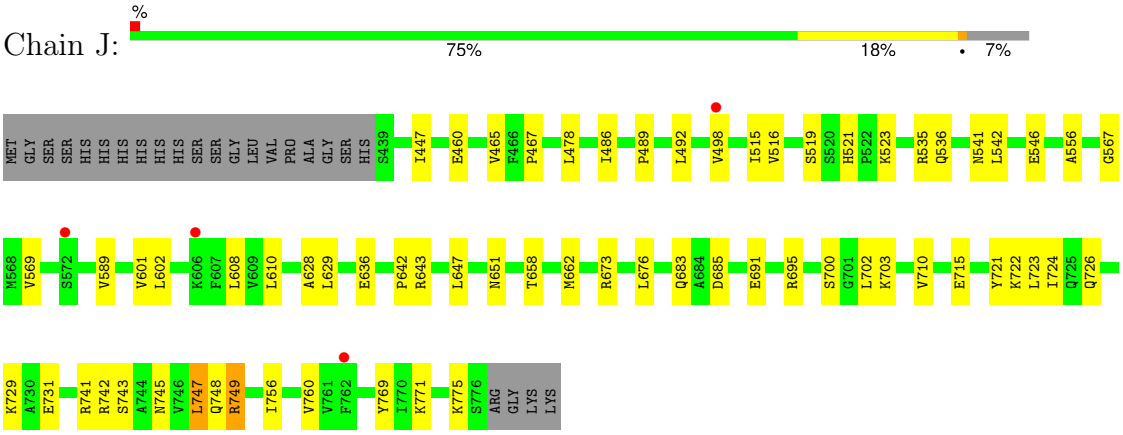
• Molecule 1: Malate dehydrogenase

Chain I:



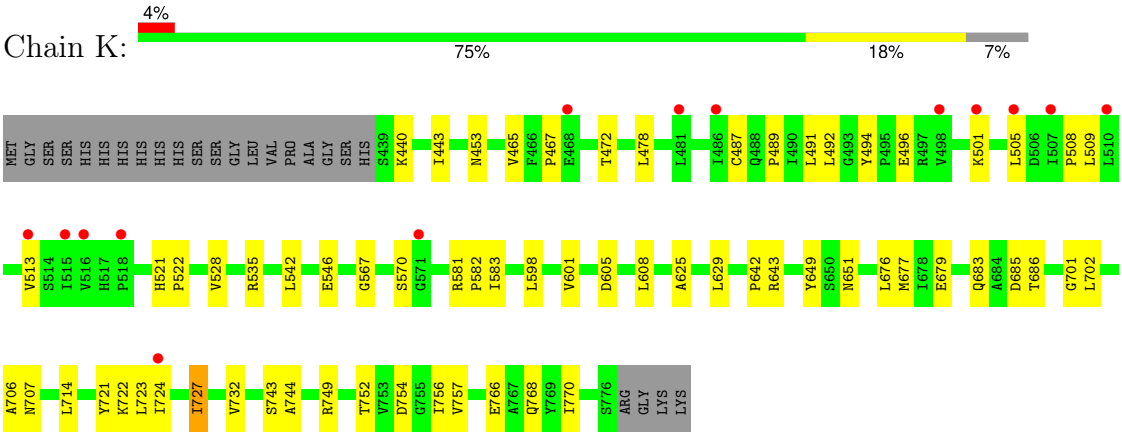
• Molecule 1: Malate dehydrogenase

Chain J:



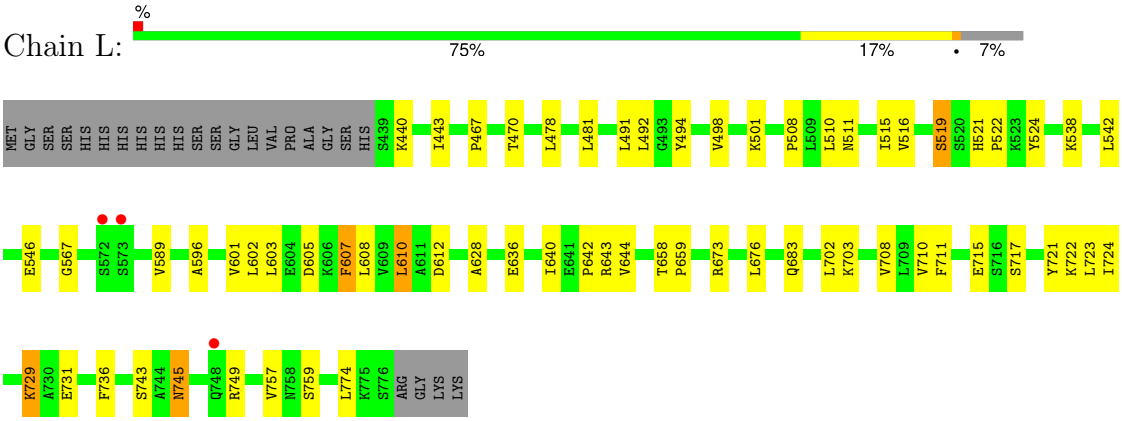
• Molecule 1: Malate dehydrogenase

Chain K:



• Molecule 1: Malate dehydrogenase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.61Å 150.81Å 282.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.78 – 3.04 102.45 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.6 (79.78-3.04) 99.8 (102.45-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.204 , 0.253 0.213 , 0.257	Depositor DCC
R_{free} test set	5586 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	89.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31317	wwPDB-VP
Average B, all atoms (Å^2)	100.0	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 39.95 % 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 2.9426e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.48	0/2642	0.67	1/3576 (0.0%)
1	B	0.49	0/2642	0.66	0/3576
1	C	0.47	0/2647	0.65	1/3583 (0.0%)
1	D	0.44	0/2659	0.64	0/3599
1	E	0.50	0/2642	0.68	1/3576 (0.0%)
1	F	0.52	2/2642 (0.1%)	0.68	0/3576
1	G	0.53	1/2642 (0.0%)	0.70	0/3576
1	H	0.51	0/2642	0.65	0/3576
1	I	0.46	0/2642	0.65	0/3576
1	J	0.51	1/2642 (0.0%)	0.68	0/3576
1	K	0.45	0/2642	0.65	1/3576 (0.0%)
1	L	0.48	0/2642	0.69	1/3576 (0.0%)
All	All	0.49	4/31726 (0.0%)	0.67	5/42942 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	460	GLU	C-N	-6.49	1.19	1.34
1	G	624	CYS	CB-SG	-5.45	1.73	1.81
1	F	624	CYS	CB-SG	-5.13	1.73	1.81
1	F	460	GLU	C-N	-5.02	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	598	LEU	CA-CB-CG	5.45	127.83	115.30
1	E	535	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	497	ARG	CB-CG-CD	-5.16	98.18	111.60
1	L	610	LEU	CA-CB-CG	5.14	127.13	115.30
1	C	725	GLN	CB-CA-C	-5.06	100.29	110.40

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	2598	0	2673	56	0
1	B	2598	0	2673	44	0
1	C	2603	0	2675	38	1
1	D	2614	0	2685	55	0
1	E	2598	0	2673	38	0
1	F	2598	0	2673	34	0
1	G	2598	0	2673	40	0
1	H	2598	0	2673	52	0
1	I	2598	0	2673	39	0
1	J	2598	0	2672	39	0
1	K	2598	0	2673	44	0
1	L	2598	0	2673	49	1
2	A	10	0	0	1	0
2	B	10	0	0	3	0
2	C	10	0	0	0	0
2	D	10	0	0	2	0
2	E	10	0	0	1	0
2	F	10	0	0	0	0
2	G	10	0	0	2	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	1	0
2	K	10	0	0	1	0
2	L	10	0	0	1	0
All	All	31317	0	32089	478	1

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 8.

The worst 5 of 478 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:A:439:SER:HA	1:A:731:GLU:OE1	1.21	1.32
1:A:439:SER:CA	1:A:731:GLU:OE1	1.76	1.31
1:B:694:GLU:HG3	1:H:704:GLY:HA2	1.51	0.93
1:L:498:VAL:HG21	1:L:515:ILE:HG21	1.56	0.88
1:H:673:ARG:NH1	1:H:675:ASP:OD2	2.10	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ASP:OD2	1:L:643:ARG:NH2[2_454]	2.19	0.01

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	336/362 (93%)	327 (97%)	9 (3%)	0	100	100
1	B	336/362 (93%)	328 (98%)	8 (2%)	0	100	100
1	C	337/362 (93%)	329 (98%)	8 (2%)	0	100	100
1	D	338/362 (93%)	330 (98%)	8 (2%)	0	100	100
1	E	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
1	F	336/362 (93%)	331 (98%)	5 (2%)	0	100	100
1	G	336/362 (93%)	328 (98%)	8 (2%)	0	100	100
1	H	336/362 (93%)	328 (98%)	8 (2%)	0	100	100
1	I	336/362 (93%)	328 (98%)	8 (2%)	0	100	100
1	J	336/362 (93%)	329 (98%)	7 (2%)	0	100	100
1	K	336/362 (93%)	327 (97%)	9 (3%)	0	100	100
1	L	336/362 (93%)	328 (98%)	8 (2%)	0	100	100
All	All	4035/4344 (93%)	3943 (98%)	92 (2%)	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	282/301 (94%)	269 (95%)	13 (5%)	27	61
1	B	282/301 (94%)	279 (99%)	3 (1%)	73	90
1	C	282/301 (94%)	278 (99%)	4 (1%)	67	86
1	D	284/301 (94%)	277 (98%)	7 (2%)	47	77
1	E	282/301 (94%)	271 (96%)	11 (4%)	32	66
1	F	282/301 (94%)	279 (99%)	3 (1%)	73	90
1	G	282/301 (94%)	269 (95%)	13 (5%)	27	61
1	H	282/301 (94%)	273 (97%)	9 (3%)	39	72
1	I	282/301 (94%)	279 (99%)	3 (1%)	73	90
1	J	282/301 (94%)	270 (96%)	12 (4%)	29	63
1	K	282/301 (94%)	279 (99%)	3 (1%)	73	90
1	L	282/301 (94%)	273 (97%)	9 (3%)	39	72
All	All	3386/3612 (94%)	3296 (97%)	90 (3%)	44	75

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	694	GLU
1	J	745	ASN
1	H	729	LYS
1	I	745	ASN
1	J	769	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	ASN

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Mol	Chain	Res	Type
1	A	562	GLN
1	K	561	ASN
1	K	562	GLN
1	L	748	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	801	-	4,4,4	0.29	0	6,6,6	0.46	0
2	SO4	E	802	-	4,4,4	0.32	0	6,6,6	0.38	0
2	SO4	A	801	-	4,4,4	0.35	0	6,6,6	0.24	0
2	SO4	L	801	-	4,4,4	0.29	0	6,6,6	0.38	0
2	SO4	D	802	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	F	801	-	4,4,4	0.32	0	6,6,6	0.29	0
2	SO4	G	801	-	4,4,4	0.36	0	6,6,6	0.40	0
2	SO4	K	801	-	4,4,4	0.31	0	6,6,6	0.32	0
2	SO4	D	801	-	4,4,4	0.31	0	6,6,6	0.29	0
2	SO4	L	802	-	4,4,4	0.36	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	802	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	H	802	-	4,4,4	0.35	0	6,6,6	0.47	0
2	SO4	I	802	-	4,4,4	0.31	0	6,6,6	0.23	0
2	SO4	J	802	-	4,4,4	0.22	0	6,6,6	0.39	0
2	SO4	H	801	-	4,4,4	0.30	0	6,6,6	0.33	0
2	SO4	C	802	-	4,4,4	0.27	0	6,6,6	0.18	0
2	SO4	K	802	-	4,4,4	0.30	0	6,6,6	0.30	0
2	SO4	A	802	-	4,4,4	0.30	0	6,6,6	0.25	0
2	SO4	E	801	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	I	801	-	4,4,4	0.25	0	6,6,6	0.47	0
2	SO4	J	801	-	4,4,4	0.38	0	6,6,6	0.18	0
2	SO4	C	801	-	4,4,4	0.28	0	6,6,6	0.35	0
2	SO4	F	802	-	4,4,4	0.30	0	6,6,6	0.14	0
2	SO4	G	802	-	4,4,4	0.40	0	6,6,6	0.40	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.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	SO4	1	0
2	E	802	SO4	1	0
2	A	801	SO4	1	0
2	L	801	SO4	1	0
2	D	802	SO4	1	0
2	G	801	SO4	1	0
2	D	801	SO4	1	0
2	B	802	SO4	2	0
2	J	802	SO4	1	0
2	K	802	SO4	1	0
2	G	802	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	460:GLU	C	461:LEU	N	1.19

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	338/362 (93%)	0.02	0 100 100	60, 95, 152, 189	0
1	B	338/362 (93%)	0.20	3 (0%) 84 62	52, 88, 149, 205	0
1	C	339/362 (93%)	0.10	4 (1%) 79 53	58, 93, 152, 209	0
1	D	340/362 (93%)	0.08	2 (0%) 89 72	56, 94, 151, 208	0
1	E	338/362 (93%)	0.20	8 (2%) 59 30	52, 89, 160, 184	0
1	F	338/362 (93%)	-0.01	1 (0%) 94 83	56, 86, 139, 173	0
1	G	338/362 (93%)	0.01	0 100 100	49, 85, 149, 202	0
1	H	338/362 (93%)	0.07	0 100 100	52, 90, 151, 192	0
1	I	338/362 (93%)	0.23	11 (3%) 46 20	56, 112, 188, 247	0
1	J	338/362 (93%)	0.13	4 (1%) 79 53	56, 86, 137, 189	0
1	K	338/362 (93%)	0.34	14 (4%) 37 15	54, 111, 196, 245	0
1	L	338/362 (93%)	0.17	3 (0%) 84 62	61, 89, 137, 182	0
All	All	4059/4344 (93%)	0.13	50 (1%) 79 53	49, 92, 161, 247	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	510	LEU	5.3
1	I	486	ILE	4.8
1	K	498	VAL	4.3
1	K	505	LEU	3.9
1	E	482	VAL	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	K	801	5/5	0.85	0.19	137,137,137,137	0
2	SO4	I	801	5/5	0.87	0.14	123,123,123,123	0
2	SO4	K	802	5/5	0.87	0.14	120,120,120,120	0
2	SO4	C	801	5/5	0.88	0.16	110,110,110,110	0
2	SO4	A	802	5/5	0.88	0.18	122,122,122,122	0
2	SO4	D	802	5/5	0.90	0.18	114,114,114,114	0
2	SO4	I	802	5/5	0.90	0.15	134,134,134,134	0
2	SO4	B	801	5/5	0.91	0.14	110,110,110,110	0
2	SO4	L	802	5/5	0.91	0.16	104,104,104,104	0
2	SO4	H	802	5/5	0.92	0.15	103,103,103,103	0
2	SO4	G	802	5/5	0.92	0.12	107,107,107,107	0
2	SO4	H	801	5/5	0.92	0.13	107,107,107,107	0
2	SO4	E	802	5/5	0.93	0.12	104,104,104,104	0
2	SO4	F	801	5/5	0.94	0.19	95,95,95,95	0
2	SO4	F	802	5/5	0.94	0.14	108,108,108,108	0
2	SO4	J	801	5/5	0.95	0.15	97,97,97,97	0
2	SO4	J	802	5/5	0.95	0.12	103,103,103,103	0
2	SO4	G	801	5/5	0.95	0.13	96,96,96,96	0
2	SO4	D	801	5/5	0.95	0.10	98,98,98,98	0
2	SO4	C	802	5/5	0.95	0.11	113,113,113,113	0
2	SO4	A	801	5/5	0.96	0.17	105,105,105,105	0
2	SO4	L	801	5/5	0.96	0.13	101,101,101,101	0
2	SO4	B	802	5/5	0.96	0.10	106,106,106,106	0
2	SO4	E	801	5/5	0.97	0.11	107,107,107,107	0

6.5 Other polymers (i)

There are no such residues in this entry.