wwPDB X-ray Structure Validation Summary Report (i)

Sep 12, 2023 – 08:44 PM EDT

PDB ID	:	4O8M
Title	:	Crystal structure of a trap periplasmic solute binding protein actinobacillus succinogenes 130z, target EFI-510004, with bound L-galactonate
Authors	:	Vetting, M.W.; Al Obaidi, N.F.; Morisco, L.L.; Wasserman, S.R.; Sojitra, S.; Stead, M.; Attonito, J.D.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hillerich, B.; Love, J.; Seidel, R.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2013-12-28
Resolution	:	1.70 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:

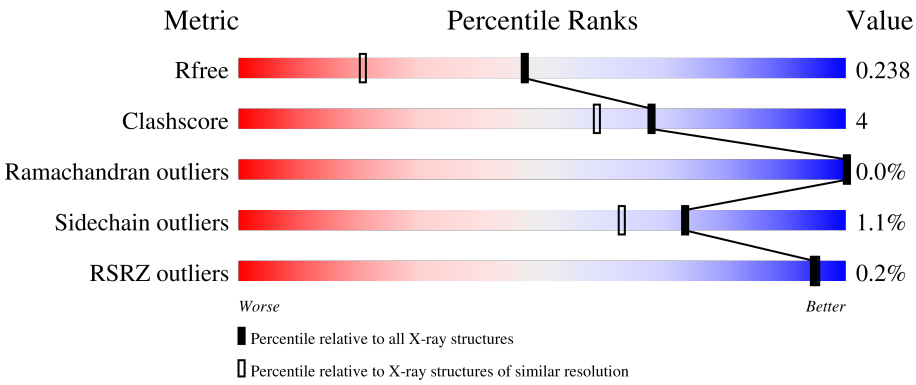
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	346	80% 7% 12%
1	B	346	82% 6% 12%
1	C	346	80% 8% 12%
1	D	346	80% 7% 13%

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Mol	Chain	Length	Quality of chain
1	E	346	80% 7% 12%
1	F	346	80% 8% 12%
1	G	346	% 79% 8% 13%
1	H	346	80% 7% 13%

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	CL	D	401	-	-	X	-
3	SO4	D	403	-	-	X	-
3	SO4	F	401	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41582 atoms, of which 18905 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 TRAP dicarboxylate transporter, DctP subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	303	4773	1530	2385	391	459	8	0	4	0
1	B	303	4732	1518	2365	387	454	8	0	1	0
1	C	303	4734	1519	2367	387	453	8	0	1	0
1	D	301	4705	1506	2354	387	450	8	0	1	0
1	E	303	4718	1514	2358	386	452	8	0	0	0
1	F	303	4732	1518	2365	387	454	8	0	1	0
1	G	302	4727	1515	2365	389	450	8	0	1	0
1	H	302	4693	1507	2346	384	448	8	0	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	ALA	-	expression tag	UNP A6VKP1
A	330	GLU	-	expression tag	UNP A6VKP1
A	331	ASN	-	expression tag	UNP A6VKP1
A	332	LEU	-	expression tag	UNP A6VKP1
A	333	TYR	-	expression tag	UNP A6VKP1
A	334	PHE	-	expression tag	UNP A6VKP1
A	335	GLN	-	expression tag	UNP A6VKP1
A	336	GLY	-	expression tag	UNP A6VKP1
A	337	HIS	-	expression tag	UNP A6VKP1
A	338	HIS	-	expression tag	UNP A6VKP1
A	339	HIS	-	expression tag	UNP A6VKP1
A	340	HIS	-	expression tag	UNP A6VKP1
A	341	HIS	-	expression tag	UNP A6VKP1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	342	HIS	-	expression tag	UNP A6VKP1
A	343	HIS	-	expression tag	UNP A6VKP1
A	344	HIS	-	expression tag	UNP A6VKP1
A	345	HIS	-	expression tag	UNP A6VKP1
A	346	HIS	-	expression tag	UNP A6VKP1
B	329	ALA	-	expression tag	UNP A6VKP1
B	330	GLU	-	expression tag	UNP A6VKP1
B	331	ASN	-	expression tag	UNP A6VKP1
B	332	LEU	-	expression tag	UNP A6VKP1
B	333	TYR	-	expression tag	UNP A6VKP1
B	334	PHE	-	expression tag	UNP A6VKP1
B	335	GLN	-	expression tag	UNP A6VKP1
B	336	GLY	-	expression tag	UNP A6VKP1
B	337	HIS	-	expression tag	UNP A6VKP1
B	338	HIS	-	expression tag	UNP A6VKP1
B	339	HIS	-	expression tag	UNP A6VKP1
B	340	HIS	-	expression tag	UNP A6VKP1
B	341	HIS	-	expression tag	UNP A6VKP1
B	342	HIS	-	expression tag	UNP A6VKP1
B	343	HIS	-	expression tag	UNP A6VKP1
B	344	HIS	-	expression tag	UNP A6VKP1
B	345	HIS	-	expression tag	UNP A6VKP1
B	346	HIS	-	expression tag	UNP A6VKP1
C	329	ALA	-	expression tag	UNP A6VKP1
C	330	GLU	-	expression tag	UNP A6VKP1
C	331	ASN	-	expression tag	UNP A6VKP1
C	332	LEU	-	expression tag	UNP A6VKP1
C	333	TYR	-	expression tag	UNP A6VKP1
C	334	PHE	-	expression tag	UNP A6VKP1
C	335	GLN	-	expression tag	UNP A6VKP1
C	336	GLY	-	expression tag	UNP A6VKP1
C	337	HIS	-	expression tag	UNP A6VKP1
C	338	HIS	-	expression tag	UNP A6VKP1
C	339	HIS	-	expression tag	UNP A6VKP1
C	340	HIS	-	expression tag	UNP A6VKP1
C	341	HIS	-	expression tag	UNP A6VKP1
C	342	HIS	-	expression tag	UNP A6VKP1
C	343	HIS	-	expression tag	UNP A6VKP1
C	344	HIS	-	expression tag	UNP A6VKP1
C	345	HIS	-	expression tag	UNP A6VKP1
C	346	HIS	-	expression tag	UNP A6VKP1
D	329	ALA	-	expression tag	UNP A6VKP1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	330	GLU	-	expression tag	UNP A6VKP1
D	331	ASN	-	expression tag	UNP A6VKP1
D	332	LEU	-	expression tag	UNP A6VKP1
D	333	TYR	-	expression tag	UNP A6VKP1
D	334	PHE	-	expression tag	UNP A6VKP1
D	335	GLN	-	expression tag	UNP A6VKP1
D	336	GLY	-	expression tag	UNP A6VKP1
D	337	HIS	-	expression tag	UNP A6VKP1
D	338	HIS	-	expression tag	UNP A6VKP1
D	339	HIS	-	expression tag	UNP A6VKP1
D	340	HIS	-	expression tag	UNP A6VKP1
D	341	HIS	-	expression tag	UNP A6VKP1
D	342	HIS	-	expression tag	UNP A6VKP1
D	343	HIS	-	expression tag	UNP A6VKP1
D	344	HIS	-	expression tag	UNP A6VKP1
D	345	HIS	-	expression tag	UNP A6VKP1
D	346	HIS	-	expression tag	UNP A6VKP1
E	329	ALA	-	expression tag	UNP A6VKP1
E	330	GLU	-	expression tag	UNP A6VKP1
E	331	ASN	-	expression tag	UNP A6VKP1
E	332	LEU	-	expression tag	UNP A6VKP1
E	333	TYR	-	expression tag	UNP A6VKP1
E	334	PHE	-	expression tag	UNP A6VKP1
E	335	GLN	-	expression tag	UNP A6VKP1
E	336	GLY	-	expression tag	UNP A6VKP1
E	337	HIS	-	expression tag	UNP A6VKP1
E	338	HIS	-	expression tag	UNP A6VKP1
E	339	HIS	-	expression tag	UNP A6VKP1
E	340	HIS	-	expression tag	UNP A6VKP1
E	341	HIS	-	expression tag	UNP A6VKP1
E	342	HIS	-	expression tag	UNP A6VKP1
E	343	HIS	-	expression tag	UNP A6VKP1
E	344	HIS	-	expression tag	UNP A6VKP1
E	345	HIS	-	expression tag	UNP A6VKP1
E	346	HIS	-	expression tag	UNP A6VKP1
F	329	ALA	-	expression tag	UNP A6VKP1
F	330	GLU	-	expression tag	UNP A6VKP1
F	331	ASN	-	expression tag	UNP A6VKP1
F	332	LEU	-	expression tag	UNP A6VKP1
F	333	TYR	-	expression tag	UNP A6VKP1
F	334	PHE	-	expression tag	UNP A6VKP1
F	335	GLN	-	expression tag	UNP A6VKP1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	336	GLY	-	expression tag	UNP A6VKP1
F	337	HIS	-	expression tag	UNP A6VKP1
F	338	HIS	-	expression tag	UNP A6VKP1
F	339	HIS	-	expression tag	UNP A6VKP1
F	340	HIS	-	expression tag	UNP A6VKP1
F	341	HIS	-	expression tag	UNP A6VKP1
F	342	HIS	-	expression tag	UNP A6VKP1
F	343	HIS	-	expression tag	UNP A6VKP1
F	344	HIS	-	expression tag	UNP A6VKP1
F	345	HIS	-	expression tag	UNP A6VKP1
F	346	HIS	-	expression tag	UNP A6VKP1
G	329	ALA	-	expression tag	UNP A6VKP1
G	330	GLU	-	expression tag	UNP A6VKP1
G	331	ASN	-	expression tag	UNP A6VKP1
G	332	LEU	-	expression tag	UNP A6VKP1
G	333	TYR	-	expression tag	UNP A6VKP1
G	334	PHE	-	expression tag	UNP A6VKP1
G	335	GLN	-	expression tag	UNP A6VKP1
G	336	GLY	-	expression tag	UNP A6VKP1
G	337	HIS	-	expression tag	UNP A6VKP1
G	338	HIS	-	expression tag	UNP A6VKP1
G	339	HIS	-	expression tag	UNP A6VKP1
G	340	HIS	-	expression tag	UNP A6VKP1
G	341	HIS	-	expression tag	UNP A6VKP1
G	342	HIS	-	expression tag	UNP A6VKP1
G	343	HIS	-	expression tag	UNP A6VKP1
G	344	HIS	-	expression tag	UNP A6VKP1
G	345	HIS	-	expression tag	UNP A6VKP1
G	346	HIS	-	expression tag	UNP A6VKP1
H	329	ALA	-	expression tag	UNP A6VKP1
H	330	GLU	-	expression tag	UNP A6VKP1
H	331	ASN	-	expression tag	UNP A6VKP1
H	332	LEU	-	expression tag	UNP A6VKP1
H	333	TYR	-	expression tag	UNP A6VKP1
H	334	PHE	-	expression tag	UNP A6VKP1
H	335	GLN	-	expression tag	UNP A6VKP1
H	336	GLY	-	expression tag	UNP A6VKP1
H	337	HIS	-	expression tag	UNP A6VKP1
H	338	HIS	-	expression tag	UNP A6VKP1
H	339	HIS	-	expression tag	UNP A6VKP1
H	340	HIS	-	expression tag	UNP A6VKP1
H	341	HIS	-	expression tag	UNP A6VKP1

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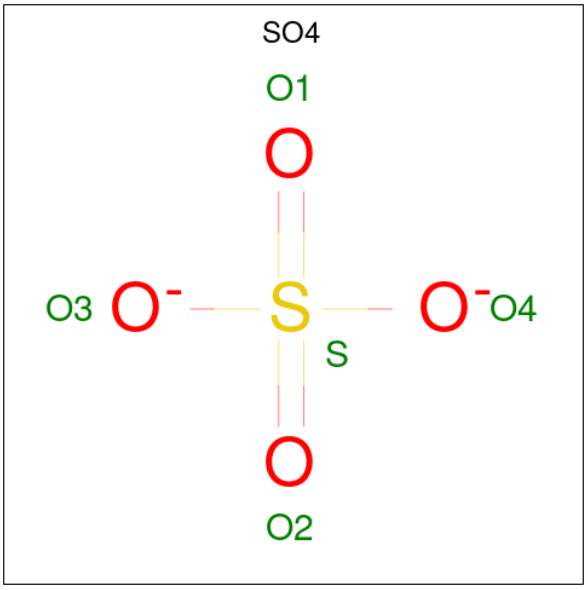
Chain	Residue	Modelled	Actual	Comment	Reference
H	342	HIS	-	expression tag	UNP A6VKP1
H	343	HIS	-	expression tag	UNP A6VKP1
H	344	HIS	-	expression tag	UNP A6VKP1
H	345	HIS	-	expression tag	UNP A6VKP1
H	346	HIS	-	expression tag	UNP A6VKP1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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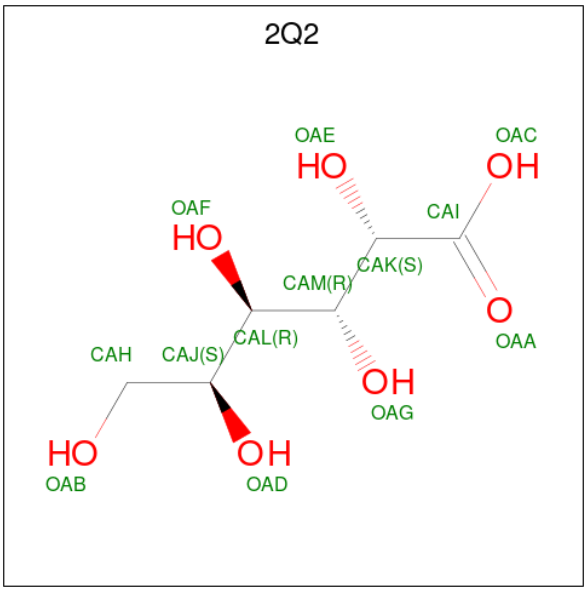
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	C	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0
			Total	O	S		
3	E	1	5	4	1	0	0
			Total	O	S		
3	F	1	5	4	1	0	0
			Total	O	S		
3	F	1	5	4	1	0	0
			Total	O	S		
3	G	1	5	4	1	0	0
			Total	O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

- Molecule 4 is L-galactonic acid (three-letter code: 2Q2) (formula: $C_6H_{12}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	6	7	0	0
4	B	1	13	6	7	0	0
4	C	1	13	6	7	0	0
4	D	1	13	6	7	0	0
4	E	1	13	6	7	0	0
4	F	1	13	6	7	0	0
4	G	1	13	6	7	0	0
4	H	1	13	6	7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	413	413	413	0	0
5	B	455	456	456	0	1
5	C	496	497	497	0	1
5	D	442	442	442	0	0

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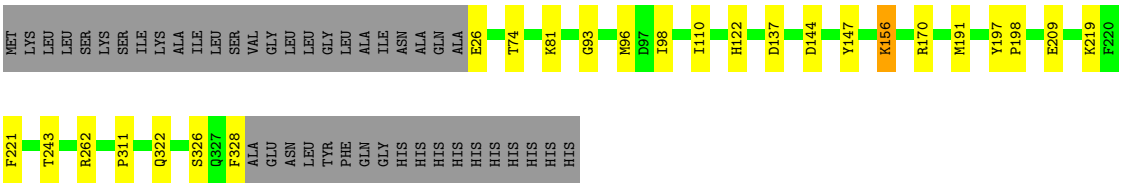
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	470	472	472	0	2
			Total	O		
5	F	401	401	401	0	0
			Total	O		
5	G	458	459	459	0	1
			Total	O		
5	H	440	441	441	0	1

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.

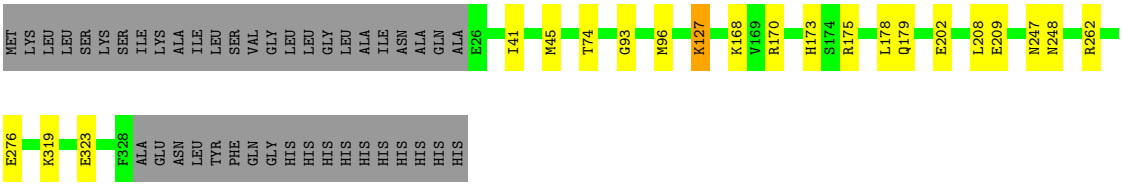
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain A:



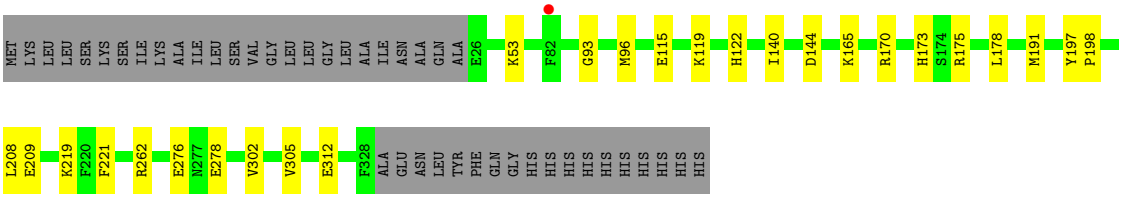
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain B:



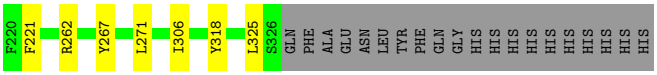
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain C:



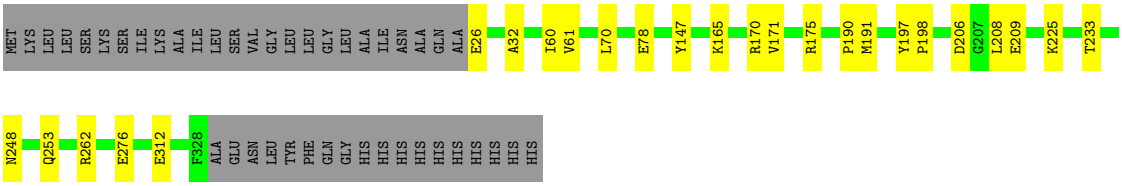
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain D:



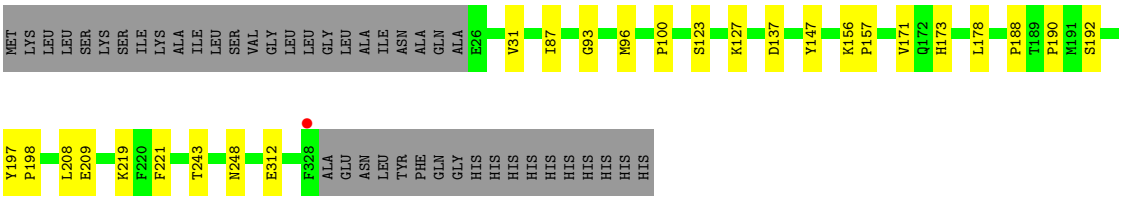
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain E:



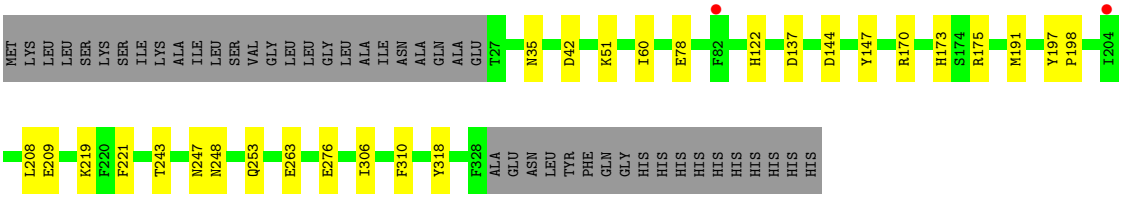
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain F:



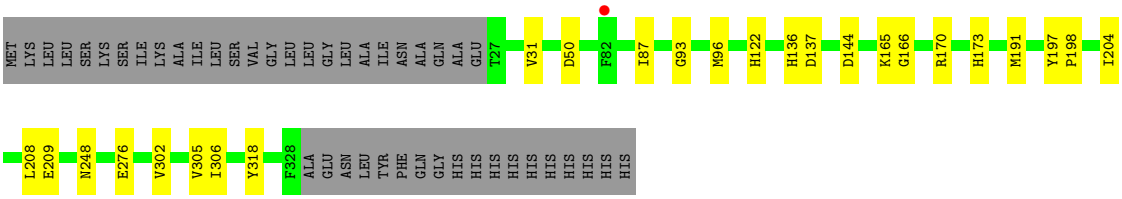
• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain G:



• Molecule 1: TRAP dicarboxylate transporter, DctP subunit

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.23Å 143.59Å 97.46Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	31.20 – 1.70 96.12 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.20-1.70) 89.4 (96.12-1.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.188 , 0.236 0.190 , 0.238	Depositor DCC
R_{free} test set	14524 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	11.3	Xtriage
Anisotropy	0.912	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41582	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 56.32 % 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 2.7829e-05. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, 2Q2

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	0/2442	0.58	0/3314
1	B	0.56	0/2421	0.61	0/3285
1	C	0.55	0/2421	0.62	0/3285
1	D	0.50	0/2404	0.58	0/3261
1	E	0.55	0/2414	0.63	0/3275
1	F	0.48	0/2421	0.57	0/3285
1	G	0.53	0/2416	0.62	0/3277
1	H	0.49	0/2401	0.59	0/3258
All	All	0.52	0/19340	0.60	0/26240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	2385	2373	22	0
1	B	2367	2365	2356	18	0
1	C	2367	2367	2358	19	0
1	D	2351	2354	2345	21	0
1	E	2360	2358	2350	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2367	2365	2356	15	0
1	G	2362	2365	2356	19	0
1	H	2347	2346	2338	16	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	D	1	0	0	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	15	0	0	2	0
3	E	5	0	0	0	0
3	F	10	0	0	2	0
3	G	20	0	0	1	0
3	H	10	0	0	1	0
4	A	13	0	11	1	0
4	B	13	0	11	0	0
4	C	13	0	11	0	0
4	D	13	0	11	0	0
4	E	13	0	11	1	0
4	F	13	0	11	1	0
4	G	13	0	11	1	0
4	H	13	0	11	0	0
5	A	413	0	0	12	0
5	B	456	0	0	10	2
5	C	497	0	0	6	1
5	D	442	0	0	6	0
5	E	472	0	0	9	0
5	F	401	0	0	4	0
5	G	459	0	0	8	1
5	H	441	0	0	6	0
All	All	22677	18905	18920	144	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 144 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:F:173:HIS:ND1	3:F:401:SO4:O4	2.05	0.90
1:G:247:ASN:ND2	5:G:781:HOH:O	2.14	0.80
1:B:247:ASN:OD1	5:B:675:HOH:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ILE:O	5:C:768:HOH:O	2.05	0.75
1:C:173:HIS:HD2	3:C:401:SO4:O3	1.72	0.72

All (2) 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)
5:B:817:HOH:O	5:G:789:HOH:O[2_655]	2.04	0.16
5:B:811:HOH:O	5:C:732:HOH:O[1_554]	2.17	0.03

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	305/346 (88%)	298 (98%)	7 (2%)	0	100	100
1	B	302/346 (87%)	297 (98%)	5 (2%)	0	100	100
1	C	302/346 (87%)	298 (99%)	4 (1%)	0	100	100
1	D	300/346 (87%)	295 (98%)	4 (1%)	1 (0%)	41	24
1	E	301/346 (87%)	297 (99%)	4 (1%)	0	100	100
1	F	302/346 (87%)	298 (99%)	4 (1%)	0	100	100
1	G	301/346 (87%)	297 (99%)	4 (1%)	0	100	100
1	H	300/346 (87%)	295 (98%)	5 (2%)	0	100	100
All	All	2413/2768 (87%)	2375 (98%)	37 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	143	PRO

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	266/297 (90%)	264 (99%)	2 (1%)	81	74
1	B	263/297 (89%)	259 (98%)	4 (2%)	65	51
1	C	263/297 (89%)	260 (99%)	3 (1%)	73	63
1	D	261/297 (88%)	258 (99%)	3 (1%)	73	63
1	E	262/297 (88%)	258 (98%)	4 (2%)	65	51
1	F	263/297 (89%)	261 (99%)	2 (1%)	81	74
1	G	262/297 (88%)	259 (99%)	3 (1%)	73	63
1	H	260/297 (88%)	258 (99%)	2 (1%)	81	74
All	All	2100/2376 (88%)	2077 (99%)	23 (1%)	73	63

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	208	LEU
1	F	209	GLU
1	F	208	LEU
1	G	191	MET
1	C	191	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	172	GLN
1	H	46	HIS
1	E	172	GLN
1	H	172	GLN
1	G	172	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)

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

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	D	402	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	G	402	-	4,4,4	0.19	0	6,6,6	0.44	0
4	2Q2	G	405	-	12,12,12	1.13	0	16,16,16	1.44	3 (18%)
3	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.52	0
3	SO4	E	401	-	4,4,4	0.20	0	6,6,6	0.29	0
3	SO4	G	404	-	4,4,4	0.15	0	6,6,6	0.16	0
3	SO4	G	403	-	4,4,4	0.11	0	6,6,6	0.35	0
3	SO4	H	402	-	4,4,4	0.17	0	6,6,6	0.34	0
4	2Q2	F	403	-	12,12,12	1.25	1 (8%)	16,16,16	0.90	0
3	SO4	D	404	-	4,4,4	0.13	0	6,6,6	0.34	0
3	SO4	A	402	-	4,4,4	0.23	0	6,6,6	0.54	0
3	SO4	F	401	-	4,4,4	0.28	0	6,6,6	0.47	0
4	2Q2	H	403	-	12,12,12	0.96	0	16,16,16	1.67	4 (25%)
3	SO4	B	402	-	4,4,4	0.40	0	6,6,6	0.42	0
4	2Q2	E	402	-	12,12,12	1.11	1 (8%)	16,16,16	1.50	3 (18%)
3	SO4	C	402	-	4,4,4	0.22	0	6,6,6	0.18	0
4	2Q2	D	405	-	12,12,12	0.89	0	16,16,16	1.45	2 (12%)
3	SO4	H	401	-	4,4,4	0.13	0	6,6,6	0.45	0
3	SO4	G	401	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	F	402	-	4,4,4	0.22	0	6,6,6	0.21	0
4	2Q2	B	403	-	12,12,12	1.23	1 (8%)	16,16,16	1.67	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	2Q2	A	403	-	12,12,12	0.85	0	16,16,16	1.52	5 (31%)
4	2Q2	C	403	-	12,12,12	0.95	0	16,16,16	1.38	4 (25%)
3	SO4	D	403	-	4,4,4	0.41	0	6,6,6	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2Q2	E	402	-	-	0/18/18/18	-
4	2Q2	F	403	-	-	0/18/18/18	-
4	2Q2	B	403	-	-	0/18/18/18	-
4	2Q2	A	403	-	-	0/18/18/18	-
4	2Q2	C	403	-	-	0/18/18/18	-
4	2Q2	D	405	-	-	0/18/18/18	-
4	2Q2	G	405	-	-	0/18/18/18	-
4	2Q2	H	403	-	-	0/18/18/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	2Q2	CAH-CAJ	2.65	1.59	1.52
4	F	403	2Q2	CAK-CAI	2.07	1.55	1.52
4	E	402	2Q2	CAL-CAM	2.03	1.57	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	402	2Q2	CAJ-CAL-CAM	-3.38	107.17	112.47
4	H	403	2Q2	CAJ-CAL-CAM	-3.00	107.77	112.47
4	H	403	2Q2	CAL-CAM-CAK	-2.93	108.40	113.60
4	B	403	2Q2	OAA-CAI-CAK	-2.80	114.26	121.63
4	B	403	2Q2	CAJ-CAL-CAM	-2.74	108.17	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	402	SO4	1	0
4	G	405	2Q2	1	0
3	C	401	SO4	1	0
4	F	403	2Q2	1	0
3	F	401	SO4	2	0
4	E	402	2Q2	1	0
3	H	401	SO4	1	0
4	A	403	2Q2	1	0
3	D	403	SO4	2	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 (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(Å^2)	Q<0.9
1	A	303/346 (87%)	-0.32	0	100	100	7, 14, 30, 45	0
1	B	303/346 (87%)	-0.40	0	100	100	5, 12, 25, 38	0
1	C	303/346 (87%)	-0.41	1 (0%)	94	94	6, 12, 24, 39	0
1	D	301/346 (86%)	-0.33	0	100	100	7, 14, 28, 41	0
1	E	303/346 (87%)	-0.40	0	100	100	5, 12, 26, 49	0
1	F	303/346 (87%)	-0.26	1 (0%)	94	94	9, 16, 32, 49	0
1	G	302/346 (87%)	-0.36	2 (0%)	87	90	7, 13, 28, 40	0
1	H	302/346 (87%)	-0.32	1 (0%)	94	94	8, 15, 29, 42	0
All	All	2420/2768 (87%)	-0.35	5 (0%)	95	95	5, 14, 29, 49	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	82	PHE	3.4
1	G	82	PHE	3.4
1	C	82	PHE	2.8
1	F	328	PHE	2.2
1	G	204	ILE	2.1

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 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, 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(Å^2)	Q<0.9
3	SO4	D	402	5/5	0.90	0.19	51,52,54,57	0
3	SO4	C	401	5/5	0.92	0.14	23,31,35,36	0
3	SO4	A	402	5/5	0.92	0.10	24,30,36,39	0
3	SO4	H	401	5/5	0.92	0.11	28,39,40,42	0
3	SO4	D	403	5/5	0.93	0.11	18,20,35,40	0
3	SO4	F	401	5/5	0.93	0.18	38,43,48,49	0
3	SO4	G	402	5/5	0.93	0.14	23,27,42,43	0
2	CL	A	401	1/1	0.93	0.11	36,36,36,36	0
3	SO4	G	401	5/5	0.94	0.22	49,50,53,59	0
2	CL	B	401	1/1	0.94	0.12	35,35,35,35	0
3	SO4	F	402	5/5	0.94	0.10	28,41,46,51	0
3	SO4	C	402	5/5	0.95	0.09	23,28,39,40	0
3	SO4	G	404	5/5	0.95	0.16	45,50,55,55	0
3	SO4	B	402	5/5	0.95	0.09	25,28,33,33	0
3	SO4	H	402	5/5	0.95	0.08	30,32,37,37	0
3	SO4	E	401	5/5	0.96	0.08	18,32,34,37	0
3	SO4	D	404	5/5	0.96	0.09	26,29,37,38	0
4	2Q2	C	403	13/13	0.97	0.08	5,7,11,14	0
4	2Q2	F	403	13/13	0.97	0.09	8,10,11,16	0
4	2Q2	H	403	13/13	0.97	0.07	6,8,12,12	0
3	SO4	G	403	5/5	0.98	0.07	26,28,30,39	0
4	2Q2	D	405	13/13	0.98	0.07	7,8,13,13	0
4	2Q2	E	402	13/13	0.98	0.09	4,7,9,10	0
4	2Q2	A	403	13/13	0.98	0.08	8,9,12,12	0
4	2Q2	G	405	13/13	0.98	0.08	6,7,11,14	0
4	2Q2	B	403	13/13	0.98	0.07	3,6,12,13	0
2	CL	D	401	1/1	0.99	0.11	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.