



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 11:13 PM GMT

PDB ID : 5EXD
Title : Crystal structure of oxalate oxidoreductase from Moorella thermoacetica bound with carboxy-di-oxido-methyl-TPP (COOM-TPP) intermediate
Authors : Gibson, M.I.; Chen, P.Y.-T.; Drennan, C.L.
Deposited on : 2015-11-23
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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

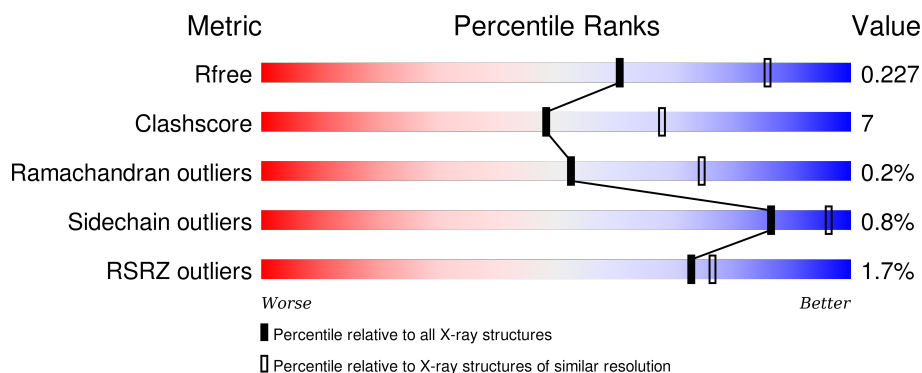
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 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	395	 77% 22% .
1	D	395	 81% 18% .
1	G	395	 79% 19% .
1	J	395	 80% 19% .
2	B	315	 77% 14% 9%

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Mol	Chain	Length	Quality of chain
2	E	315	
2	H	315	
2	K	315	
3	C	314	
3	F	314	
3	I	314	
3	L	314	

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
4	SF4	C	401	-	-	X	-
4	SF4	F	401	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30592 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 Oxalate oxidoreductase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3060	1948	522	576	14			
1	D	394	Total	C	N	O	S	0	0	0
			3055	1944	523	574	14			
1	G	394	Total	C	N	O	S	0	0	0
			3058	1945	523	576	14			
1	J	394	Total	C	N	O	S	0	0	0
			3058	1947	521	576	14			

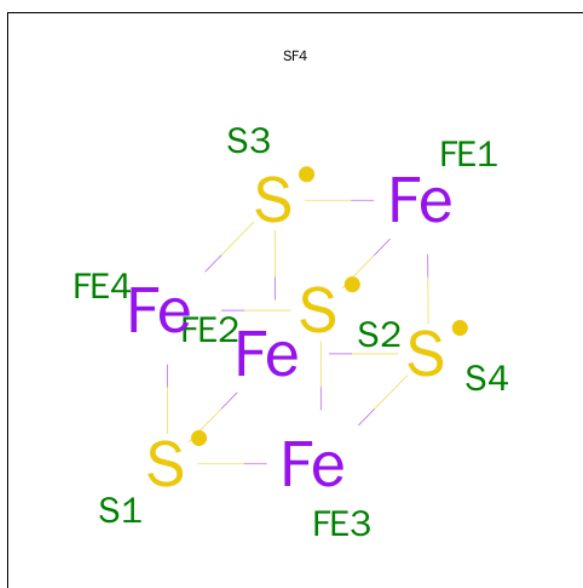
- Molecule 2 is a protein called Oxalate oxidoreductase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	0	0
			2162	1369	361	417	15			
2	E	295	Total	C	N	O	S	0	0	0
			2180	1369	368	429	14			
2	H	291	Total	C	N	O	S	0	0	0
			2200	1390	371	424	15			
2	K	280	Total	C	N	O	S	0	0	0
			2091	1317	352	407	15			

- Molecule 3 is a protein called Oxalate oxidoreductase subunit beta.

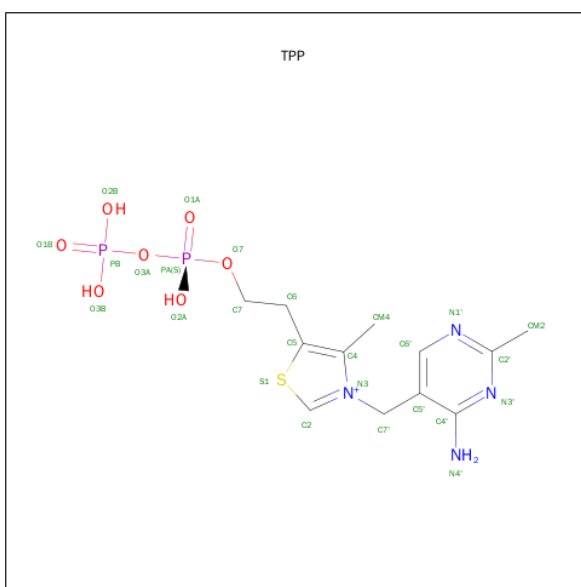
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	312	Total	C	N	O	S	0	0	0
			2393	1535	409	432	17			
3	F	310	Total	C	N	O	S	0	0	0
			2371	1522	405	427	17			
3	I	309	Total	C	N	O	S	0	0	0
			2362	1516	402	428	16			
3	L	310	Total	C	N	O	S	0	0	0
			2375	1524	405	429	17			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	F	1	Total	Fe	S	0	0
			8	4	4		
4	H	1	Total	Fe	S	0	0
			8	4	4		
4	H	1	Total	Fe	S	0	0
			8	4	4		
4	I	1	Total	Fe	S	0	0
			8	4	4		
4	K	1	Total	Fe	S	0	0
			8	4	4		
4	K	1	Total	Fe	S	0	0
			8	4	4		
4	L	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).

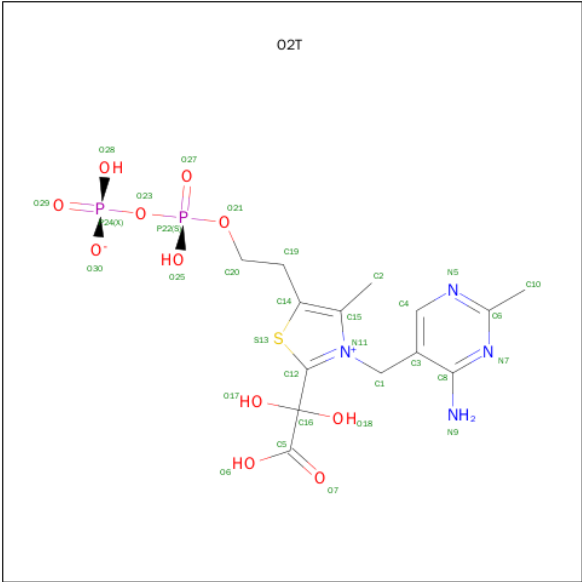


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
5	I	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0
5	L	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Mg	0	0
			1	1		
6	L	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is [2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-2-[1,1,2-tris(oxidanyl)-2-oxidanylidene-ethyl]-1,3-thiazol-3-ium-5-yl]ethoxy-oxidanyl-phosphoryl] hydrogen phosphate (three-letter code: O2T) (formula: C₁₄H₂₀N₄O₁₁P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	N	O	P	S	
			32	14	4	11	2	1	0

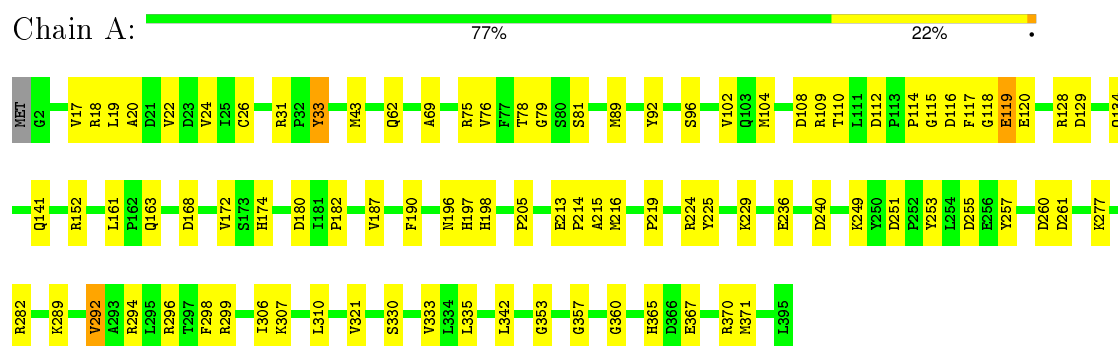
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		
8	C	1	Total	O	0	0
			1	1		
8	D	1	Total	O	0	0
			1	1		
8	F	4	Total	O	0	0
			4	4		
8	G	2	Total	O	0	0
			2	2		
8	H	1	Total	O	0	0
			1	1		
8	I	4	Total	O	0	0
			4	4		
8	L	1	Total	O	0	0
			1	1		

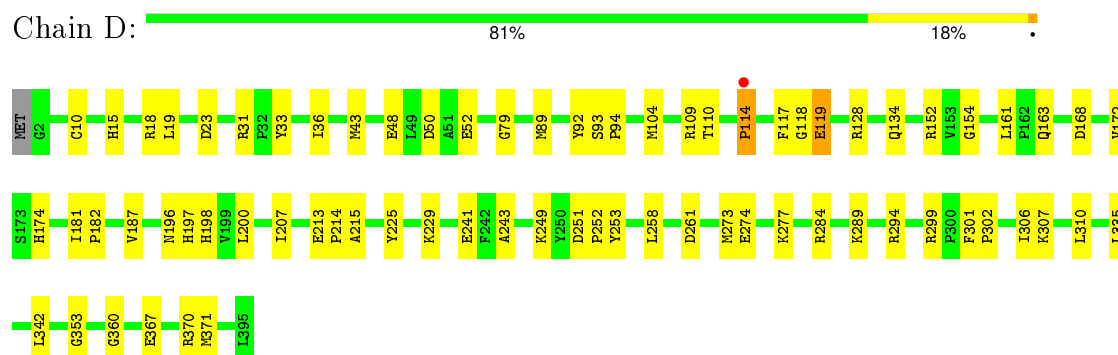
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

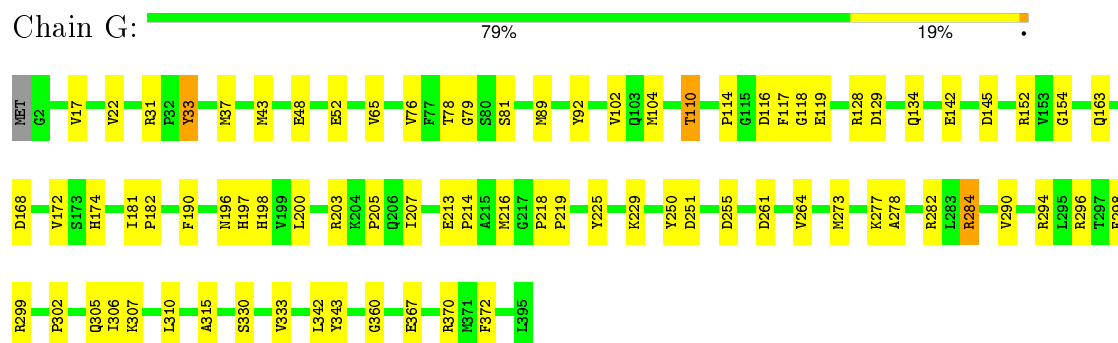
- Molecule 1: Oxalate oxidoreductase subunit alpha



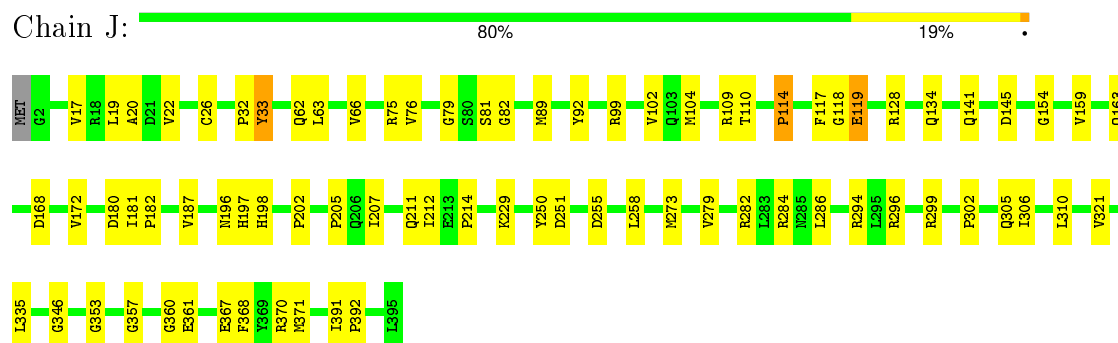
- Molecule 1: Oxalate oxidoreductase subunit alpha



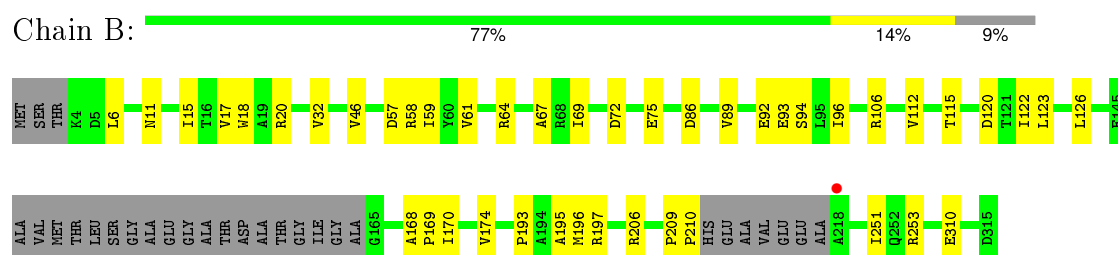
- Molecule 1: Oxalate oxidoreductase subunit alpha



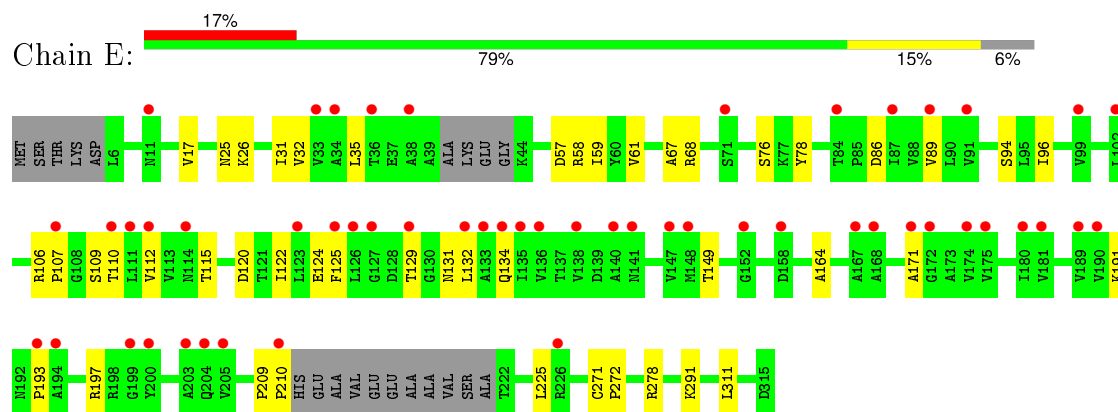
- Molecule 1: Oxalate oxidoreductase subunit alpha



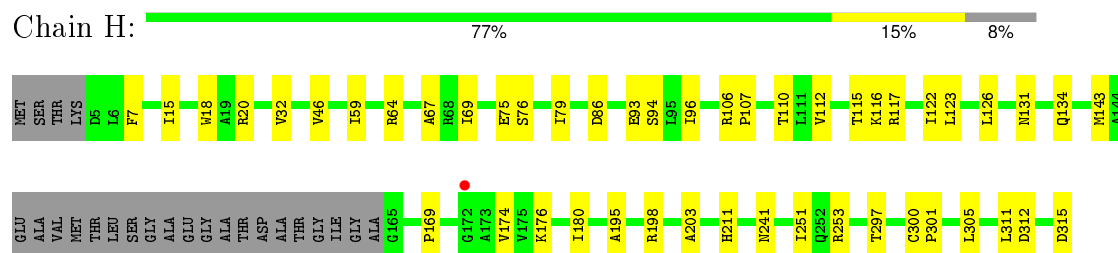
- Molecule 2: Oxalate oxidoreductase subunit delta



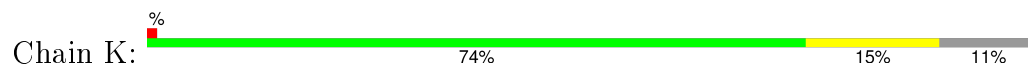
- Molecule 2: Oxalate oxidoreductase subunit delta

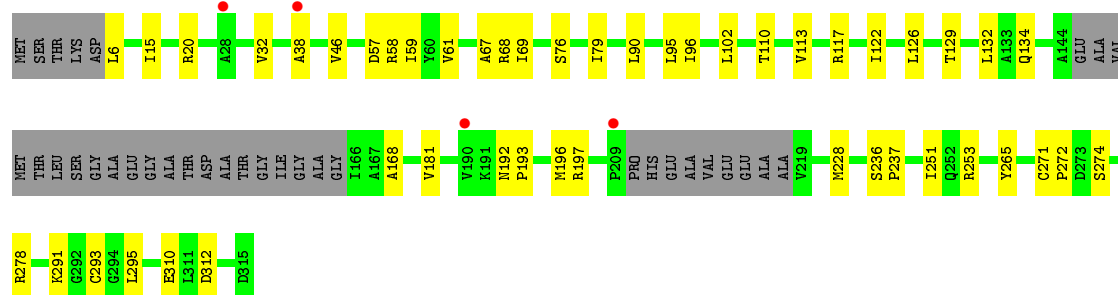


- Molecule 2: Oxalate oxidoreductase subunit delta

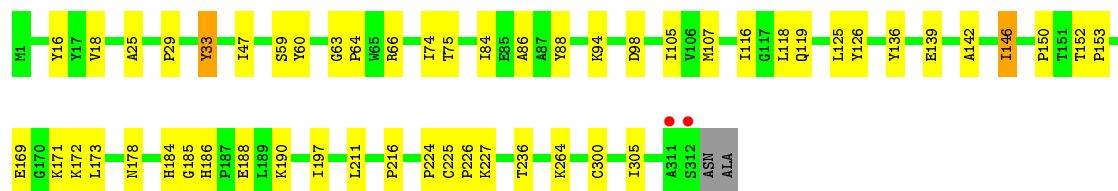
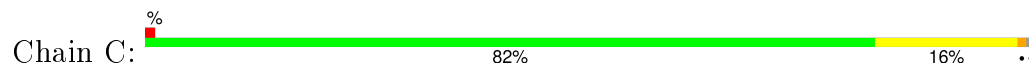


- Molecule 2: Oxalate oxidoreductase subunit delta

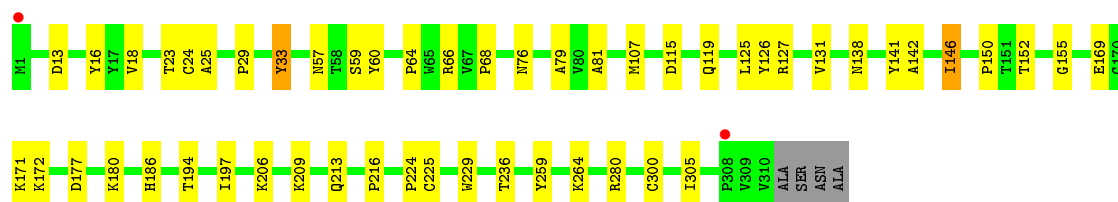
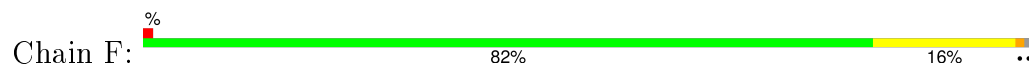




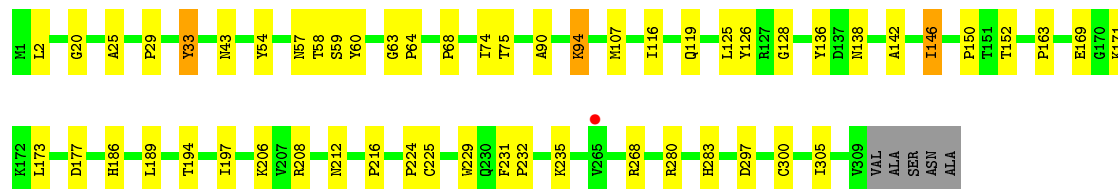
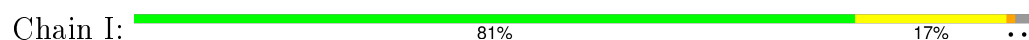
- Molecule 3: Oxalate oxidoreductase subunit beta



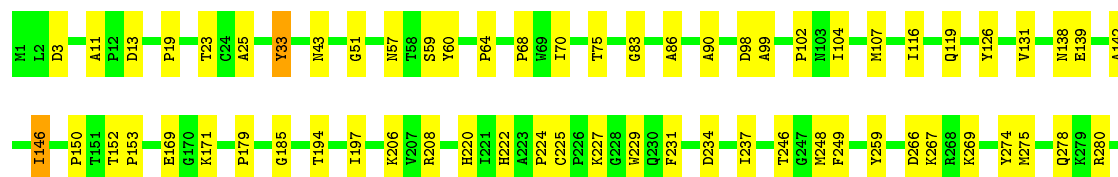
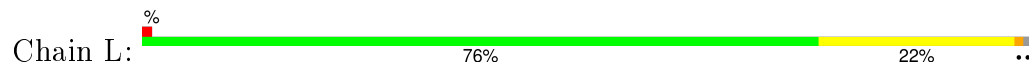
- Molecule 3: Oxalate oxidoreductase subunit beta

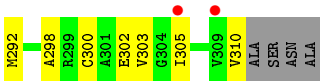


- Molecule 3: Oxalate oxidoreductase subunit beta



- Molecule 3: Oxalate oxidoreductase subunit beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	138.43Å 138.43Å 217.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.50 48.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.94-2.50) 93.2 (48.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.196 , 0.229 0.196 , 0.227	Depositor DCC
R_{free} test set	6523 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.947	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 6.5	EDS
Estimated twinning fraction	0.640 for h,-k,-l 0.328 for h,-k,-l	Xtriage
Reported twinning fraction	0.640 for h,-k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 131805 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30592	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, SF4, O2T, TPP

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	0.23	0/3132	0.41	0/4248
1	D	0.23	0/3127	0.40	0/4243
1	G	0.24	0/3130	0.42	0/4247
1	J	0.24	0/3130	0.41	0/4246
2	B	0.22	0/2201	0.42	0/3003
2	E	0.22	0/2219	0.41	0/3036
2	H	0.22	0/2241	0.42	0/3059
2	K	0.21	0/2129	0.41	0/2911
3	C	0.24	0/2458	0.41	0/3339
3	F	0.23	0/2436	0.41	0/3312
3	I	0.23	0/2427	0.40	0/3300
3	L	0.23	0/2440	0.41	0/3317
All	All	0.23	0/31070	0.41	0/42261

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

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	3060	0	2992	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3055	0	2979	47	0
1	G	3058	0	2981	61	0
1	J	3058	0	2985	54	0
2	B	2162	0	2149	25	0
2	E	2180	0	2102	29	0
2	H	2200	0	2182	28	0
2	K	2091	0	2019	35	0
3	C	2393	0	2394	40	0
3	F	2371	0	2360	38	0
3	I	2362	0	2346	41	0
3	L	2375	0	2364	48	0
4	B	16	0	0	0	0
4	C	8	0	0	2	0
4	E	16	0	0	0	0
4	F	8	0	0	2	0
4	H	16	0	0	0	0
4	I	8	0	0	1	0
4	K	16	0	0	0	0
4	L	8	0	0	1	0
5	C	26	0	16	2	0
5	I	26	0	16	1	0
5	L	26	0	16	1	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	L	1	0	0	0	0
7	F	32	0	2	2	0
8	A	3	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	4	0	0	1	0
8	G	2	0	0	0	0
8	H	1	0	0	0	0
8	I	4	0	0	0	0
8	L	1	0	0	0	0
All	All	30592	0	29903	438	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 7.

The worst 5 of 438 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)
2:E:164:ALA:HA	2:E:191:LYS:HB2	1.67	0.76
1:G:261:ASP:OD1	1:G:284:ARG:NH2	2.18	0.76
3:C:94:LYS:NZ	1:D:50:ASP:O	2.18	0.75
2:K:117:ARG:NH1	2:K:312:ASP:OD1	2.20	0.74
1:G:284:ARG:NH1	1:G:290:VAL:O	2.21	0.74

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	392/395 (99%)	378 (96%)	14 (4%)	0	100	100
1	D	392/395 (99%)	379 (97%)	12 (3%)	1 (0%)	46	68
1	G	392/395 (99%)	378 (96%)	14 (4%)	0	100	100
1	J	392/395 (99%)	378 (96%)	13 (3%)	1 (0%)	46	68
2	B	280/315 (89%)	272 (97%)	8 (3%)	0	100	100
2	E	289/315 (92%)	280 (97%)	9 (3%)	0	100	100
2	H	287/315 (91%)	277 (96%)	10 (4%)	0	100	100
2	K	274/315 (87%)	267 (97%)	7 (3%)	0	100	100
3	C	310/314 (99%)	301 (97%)	8 (3%)	1 (0%)	46	68
3	F	308/314 (98%)	299 (97%)	8 (3%)	1 (0%)	46	68
3	I	307/314 (98%)	296 (96%)	10 (3%)	1 (0%)	46	68
3	L	308/314 (98%)	298 (97%)	9 (3%)	1 (0%)	46	68
All	All	3931/4096 (96%)	3803 (97%)	122 (3%)	6 (0%)	52	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	146	ILE

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Mol	Chain	Res	Type
3	F	146	ILE
3	I	146	ILE
3	C	146	ILE
1	D	114	PRO

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	319/322 (99%)	313 (98%)	6 (2%)	65	87
1	D	317/322 (98%)	313 (99%)	4 (1%)	76	92
1	G	318/322 (99%)	312 (98%)	6 (2%)	65	87
1	J	318/322 (99%)	315 (99%)	3 (1%)	84	95
2	B	233/256 (91%)	233 (100%)	0	100	100
2	E	227/256 (89%)	227 (100%)	0	100	100
2	H	236/256 (92%)	235 (100%)	1 (0%)	93	98
2	K	219/256 (86%)	219 (100%)	0	100	100
3	C	249/250 (100%)	248 (100%)	1 (0%)	93	98
3	F	245/250 (98%)	244 (100%)	1 (0%)	93	98
3	I	244/250 (98%)	242 (99%)	2 (1%)	86	96
3	L	246/250 (98%)	244 (99%)	2 (1%)	86	96
All	All	3171/3312 (96%)	3145 (99%)	26 (1%)	86	96

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	33	TYR
1	G	119	GLU
3	L	33	TYR
1	G	33	TYR
1	G	110	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	178	ASN
2	E	11	ASN
2	E	131	ASN
2	K	204	GLN

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 ⓘ

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z > 2$
4	SF4	B	401	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	402	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	C	401	3	0,12,12	0.00	-	0,24,24	0.00	-
5	TPP	C	402	6	20,27,27	1.89	5 (25%)	27,40,40	1.42	4 (14%)
4	SF4	E	401	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	E	402	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	F	401	3	0,12,12	0.00	-	0,24,24	0.00	-
7	O2T	F	402[A]	-	22,33,33	1.69	3 (13%)	30,51,51	1.30	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	H	401	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	H	402	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	I	401	3	0,12,12	0.00	-	0,24,24	0.00	-
5	TPP	I	402	6	20,27,27	1.93	5 (25%)	27,40,40	1.36	5 (18%)
4	SF4	K	401	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	K	402	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	L	401	3	0,12,12	0.00	-	0,24,24	0.00	-
5	TPP	L	402	6	20,27,27	1.88	5 (25%)	27,40,40	1.46	7 (25%)

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	SF4	B	401	2	-	0/0/48/48	0/6/5/5
4	SF4	B	402	2	-	0/0/48/48	0/6/5/5
4	SF4	C	401	3	-	0/0/48/48	0/6/5/5
5	TPP	C	402	6	-	0/16/17/17	0/2/2/2
4	SF4	E	401	2	-	0/0/48/48	0/6/5/5
4	SF4	E	402	2	-	0/0/48/48	0/6/5/5
4	SF4	F	401	3	-	0/0/48/48	0/6/5/5
7	O2T	F	402[A]	-	-	0/16/29/29	0/2/2/2
4	SF4	H	401	2	-	0/0/48/48	0/6/5/5
4	SF4	H	402	2	-	0/0/48/48	0/6/5/5
4	SF4	I	401	3	-	0/0/48/48	0/6/5/5
5	TPP	I	402	6	-	0/16/17/17	0/2/2/2
4	SF4	K	401	2	-	0/0/48/48	0/6/5/5
4	SF4	K	402	2	-	0/0/48/48	0/6/5/5
4	SF4	L	401	3	-	0/0/48/48	0/6/5/5
5	TPP	L	402	6	-	0/16/17/17	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	402	TPP	C4-N3	-4.61	1.35	1.39
5	C	402	TPP	C4-N3	-4.44	1.35	1.39
5	L	402	TPP	C4-N3	-4.25	1.36	1.39
5	I	402	TPP	C7'-N3	-3.36	1.42	1.48
5	C	402	TPP	C7'-N3	-3.35	1.42	1.48

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	402[A]	O2T	N5-C6-N7	-2.72	120.39	125.50
5	I	402	TPP	C5'-C6'-N1'	-2.48	119.52	123.86
5	C	402	TPP	C5'-C6'-N1'	-2.47	119.54	123.86
5	L	402	TPP	C5'-C6'-N1'	-2.43	119.61	123.86
5	L	402	TPP	C6-C5-C4	-2.40	124.66	127.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	SF4	2	0
5	C	402	TPP	2	0
4	F	401	SF4	2	0
7	F	402[A]	O2T	2	0
4	I	401	SF4	1	0
5	I	402	TPP	1	0
4	L	401	SF4	1	0
5	L	402	TPP	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, 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	394/395 (99%)	-0.39	0 100 100	21, 32, 47, 55	0
1	D	394/395 (99%)	-0.38	1 (0%) 94 95	22, 35, 47, 52	0
1	G	394/395 (99%)	-0.54	0 100 100	19, 25, 33, 44	0
1	J	394/395 (99%)	-0.48	0 100 100	21, 30, 38, 44	0
2	B	286/315 (90%)	-0.17	1 (0%) 94 95	24, 42, 58, 69	0
2	E	295/315 (93%)	0.80	53 (17%) 2 2	26, 66, 105, 117	0
2	H	291/315 (92%)	-0.21	1 (0%) 94 95	27, 40, 56, 61	0
2	K	280/315 (88%)	0.06	4 (1%) 78 80	26, 54, 76, 82	0
3	C	312/314 (99%)	-0.48	2 (0%) 90 91	20, 25, 38, 51	0
3	F	310/314 (98%)	-0.44	2 (0%) 90 91	20, 29, 41, 54	0
3	I	309/314 (98%)	-0.33	1 (0%) 94 95	25, 33, 45, 62	0
3	L	310/314 (98%)	-0.31	2 (0%) 90 91	25, 35, 47, 60	0
All	All	3969/4096 (96%)	-0.26	67 (1%) 73 76	19, 33, 67, 117	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	205	VAL	6.7
2	E	110	THR	5.6
2	E	138	VAL	5.6
2	E	126	LEU	5.3
2	B	218	ALA	5.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SF4	E	401	8/8	0.98	0.14	1.02	27,32,34,34	0
7	O2T	F	402[A]	32/32	0.97	0.13	0.62	24,28,31,31	6
4	SF4	B	401	8/8	0.98	0.13	0.35	23,25,28,28	0
4	SF4	H	401	8/8	0.98	0.13	0.32	26,30,34,35	0
5	TPP	L	402	26/26	0.97	0.12	0.25	25,31,33,33	0
6	MG	L	403	1/1	0.96	0.12	-0.03	32,32,32,32	0
4	SF4	H	402	8/8	0.98	0.12	-0.08	31,34,35,36	0
4	SF4	B	402	8/8	0.97	0.11	-0.11	28,29,33,34	0
4	SF4	I	401	8/8	0.98	0.12	-0.12	25,28,31,32	0
5	TPP	I	402	26/26	0.97	0.11	-0.26	22,26,27,28	0
5	TPP	C	402	26/26	0.97	0.11	-0.32	19,22,23,24	0
6	MG	I	403	1/1	0.98	0.11	-0.38	26,26,26,26	0
4	SF4	C	401	8/8	0.98	0.09	-0.55	21,23,24,25	0
4	SF4	L	401	8/8	0.97	0.11	-0.74	31,31,33,36	0
4	SF4	E	402	8/8	0.98	0.11	-0.80	30,32,33,35	0
4	SF4	K	401	8/8	0.98	0.11	-0.83	33,35,37,37	0
4	SF4	F	401	8/8	0.98	0.10	-0.84	24,30,31,31	0
4	SF4	K	402	8/8	0.99	0.09	-1.44	31,33,35,37	0
6	MG	F	403	1/1	0.98	0.09	-1.63	26,26,26,26	0
6	MG	C	403	1/1	0.97	0.09	-1.89	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.