



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 7, 2017 – 08:37 AM EDT

PDB ID : 5O30
Title : Crystal structure of the novel halohydrin dehalogenase HheG
Authors : Diederich, C.; Schallmeyer, A.; Blankenfeldt, W.
Deposited on : unknown
Resolution : 2.30 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

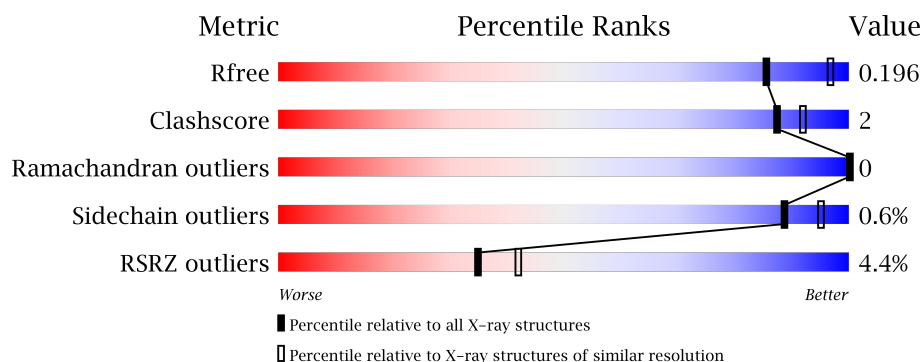
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	282	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>9%</div> </div> </div>
1	B	282	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> </div> </div>
1	C	282	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> </div> </div>
1	D	282	<div> <div></div> <div> <div></div> <div>89%</div> <div>9%</div> </div> </div>
1	E	282	<div> <div></div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	282	<div><div></div><div>90%</div><div></div><div>9%</div></div>
1	G	282	<div><div>4%</div><div></div><div>84%</div><div>7%</div><div>9%</div></div>
1	H	282	<div><div>15%</div><div></div><div>85%</div><div>6%</div><div>9%</div></div>
1	I	282	<div><div>7%</div><div></div><div>83%</div><div>8%</div><div>9%</div></div>
1	J	282	<div><div>7%</div><div></div><div>81%</div><div>10%</div><div>9%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 38900 atoms, of which 18637 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total	C	H	N	O	S	0	5	0
			3796	1193	1883	340	363	17			
1	B	258	Total	C	H	N	O	S	0	3	0
			3793	1192	1880	339	366	16			
1	C	257	Total	C	H	N	O	S	0	5	0
			3809	1195	1889	346	365	14			
1	D	257	Total	C	H	N	O	S	0	3	0
			3775	1186	1869	340	366	14			
1	E	257	Total	C	H	N	O	S	0	1	0
			3778	1184	1874	341	365	14			
1	F	258	Total	C	H	N	O	S	0	3	0
			3825	1198	1902	343	366	16			
1	G	257	Total	C	H	N	O	S	0	2	0
			3733	1177	1842	335	366	13			
1	H	257	Total	C	H	N	O	S	0	1	0
			3710	1171	1831	336	360	12			
1	I	257	Total	C	H	N	O	S	0	0	0
			3683	1165	1815	333	358	12			
1	J	257	Total	C	H	N	O	S	0	0	0
			3721	1173	1838	334	364	12			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP M5A5Y8
A	-18	GLY	-	expression tag	UNP M5A5Y8
A	-17	SER	-	expression tag	UNP M5A5Y8
A	-16	SER	-	expression tag	UNP M5A5Y8
A	-15	HIS	-	expression tag	UNP M5A5Y8
A	-14	HIS	-	expression tag	UNP M5A5Y8
A	-13	HIS	-	expression tag	UNP M5A5Y8
A	-12	HIS	-	expression tag	UNP M5A5Y8
A	-11	HIS	-	expression tag	UNP M5A5Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP M5A5Y8
A	-9	SER	-	expression tag	UNP M5A5Y8
A	-8	SER	-	expression tag	UNP M5A5Y8
A	-7	GLY	-	expression tag	UNP M5A5Y8
A	-6	LEU	-	expression tag	UNP M5A5Y8
A	-5	VAL	-	expression tag	UNP M5A5Y8
A	-4	PRO	-	expression tag	UNP M5A5Y8
A	-3	ARG	-	expression tag	UNP M5A5Y8
A	-2	GLY	-	expression tag	UNP M5A5Y8
A	-1	SER	-	expression tag	UNP M5A5Y8
A	0	HIS	-	expression tag	UNP M5A5Y8
B	-19	MET	-	initiating methionine	UNP M5A5Y8
B	-18	GLY	-	expression tag	UNP M5A5Y8
B	-17	SER	-	expression tag	UNP M5A5Y8
B	-16	SER	-	expression tag	UNP M5A5Y8
B	-15	HIS	-	expression tag	UNP M5A5Y8
B	-14	HIS	-	expression tag	UNP M5A5Y8
B	-13	HIS	-	expression tag	UNP M5A5Y8
B	-12	HIS	-	expression tag	UNP M5A5Y8
B	-11	HIS	-	expression tag	UNP M5A5Y8
B	-10	HIS	-	expression tag	UNP M5A5Y8
B	-9	SER	-	expression tag	UNP M5A5Y8
B	-8	SER	-	expression tag	UNP M5A5Y8
B	-7	GLY	-	expression tag	UNP M5A5Y8
B	-6	LEU	-	expression tag	UNP M5A5Y8
B	-5	VAL	-	expression tag	UNP M5A5Y8
B	-4	PRO	-	expression tag	UNP M5A5Y8
B	-3	ARG	-	expression tag	UNP M5A5Y8
B	-2	GLY	-	expression tag	UNP M5A5Y8
B	-1	SER	-	expression tag	UNP M5A5Y8
B	0	HIS	-	expression tag	UNP M5A5Y8
C	-19	MET	-	initiating methionine	UNP M5A5Y8
C	-18	GLY	-	expression tag	UNP M5A5Y8
C	-17	SER	-	expression tag	UNP M5A5Y8
C	-16	SER	-	expression tag	UNP M5A5Y8
C	-15	HIS	-	expression tag	UNP M5A5Y8
C	-14	HIS	-	expression tag	UNP M5A5Y8
C	-13	HIS	-	expression tag	UNP M5A5Y8
C	-12	HIS	-	expression tag	UNP M5A5Y8
C	-11	HIS	-	expression tag	UNP M5A5Y8
C	-10	HIS	-	expression tag	UNP M5A5Y8
C	-9	SER	-	expression tag	UNP M5A5Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP M5A5Y8
C	-7	GLY	-	expression tag	UNP M5A5Y8
C	-6	LEU	-	expression tag	UNP M5A5Y8
C	-5	VAL	-	expression tag	UNP M5A5Y8
C	-4	PRO	-	expression tag	UNP M5A5Y8
C	-3	ARG	-	expression tag	UNP M5A5Y8
C	-2	GLY	-	expression tag	UNP M5A5Y8
C	-1	SER	-	expression tag	UNP M5A5Y8
C	0	HIS	-	expression tag	UNP M5A5Y8
D	-19	MET	-	initiating methionine	UNP M5A5Y8
D	-18	GLY	-	expression tag	UNP M5A5Y8
D	-17	SER	-	expression tag	UNP M5A5Y8
D	-16	SER	-	expression tag	UNP M5A5Y8
D	-15	HIS	-	expression tag	UNP M5A5Y8
D	-14	HIS	-	expression tag	UNP M5A5Y8
D	-13	HIS	-	expression tag	UNP M5A5Y8
D	-12	HIS	-	expression tag	UNP M5A5Y8
D	-11	HIS	-	expression tag	UNP M5A5Y8
D	-10	HIS	-	expression tag	UNP M5A5Y8
D	-9	SER	-	expression tag	UNP M5A5Y8
D	-8	SER	-	expression tag	UNP M5A5Y8
D	-7	GLY	-	expression tag	UNP M5A5Y8
D	-6	LEU	-	expression tag	UNP M5A5Y8
D	-5	VAL	-	expression tag	UNP M5A5Y8
D	-4	PRO	-	expression tag	UNP M5A5Y8
D	-3	ARG	-	expression tag	UNP M5A5Y8
D	-2	GLY	-	expression tag	UNP M5A5Y8
D	-1	SER	-	expression tag	UNP M5A5Y8
D	0	HIS	-	expression tag	UNP M5A5Y8
E	-19	MET	-	initiating methionine	UNP M5A5Y8
E	-18	GLY	-	expression tag	UNP M5A5Y8
E	-17	SER	-	expression tag	UNP M5A5Y8
E	-16	SER	-	expression tag	UNP M5A5Y8
E	-15	HIS	-	expression tag	UNP M5A5Y8
E	-14	HIS	-	expression tag	UNP M5A5Y8
E	-13	HIS	-	expression tag	UNP M5A5Y8
E	-12	HIS	-	expression tag	UNP M5A5Y8
E	-11	HIS	-	expression tag	UNP M5A5Y8
E	-10	HIS	-	expression tag	UNP M5A5Y8
E	-9	SER	-	expression tag	UNP M5A5Y8
E	-8	SER	-	expression tag	UNP M5A5Y8
E	-7	GLY	-	expression tag	UNP M5A5Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	LEU	-	expression tag	UNP M5A5Y8
E	-5	VAL	-	expression tag	UNP M5A5Y8
E	-4	PRO	-	expression tag	UNP M5A5Y8
E	-3	ARG	-	expression tag	UNP M5A5Y8
E	-2	GLY	-	expression tag	UNP M5A5Y8
E	-1	SER	-	expression tag	UNP M5A5Y8
E	0	HIS	-	expression tag	UNP M5A5Y8
F	-19	MET	-	initiating methionine	UNP M5A5Y8
F	-18	GLY	-	expression tag	UNP M5A5Y8
F	-17	SER	-	expression tag	UNP M5A5Y8
F	-16	SER	-	expression tag	UNP M5A5Y8
F	-15	HIS	-	expression tag	UNP M5A5Y8
F	-14	HIS	-	expression tag	UNP M5A5Y8
F	-13	HIS	-	expression tag	UNP M5A5Y8
F	-12	HIS	-	expression tag	UNP M5A5Y8
F	-11	HIS	-	expression tag	UNP M5A5Y8
F	-10	HIS	-	expression tag	UNP M5A5Y8
F	-9	SER	-	expression tag	UNP M5A5Y8
F	-8	SER	-	expression tag	UNP M5A5Y8
F	-7	GLY	-	expression tag	UNP M5A5Y8
F	-6	LEU	-	expression tag	UNP M5A5Y8
F	-5	VAL	-	expression tag	UNP M5A5Y8
F	-4	PRO	-	expression tag	UNP M5A5Y8
F	-3	ARG	-	expression tag	UNP M5A5Y8
F	-2	GLY	-	expression tag	UNP M5A5Y8
F	-1	SER	-	expression tag	UNP M5A5Y8
F	0	HIS	-	expression tag	UNP M5A5Y8
G	-19	MET	-	initiating methionine	UNP M5A5Y8
G	-18	GLY	-	expression tag	UNP M5A5Y8
G	-17	SER	-	expression tag	UNP M5A5Y8
G	-16	SER	-	expression tag	UNP M5A5Y8
G	-15	HIS	-	expression tag	UNP M5A5Y8
G	-14	HIS	-	expression tag	UNP M5A5Y8
G	-13	HIS	-	expression tag	UNP M5A5Y8
G	-12	HIS	-	expression tag	UNP M5A5Y8
G	-11	HIS	-	expression tag	UNP M5A5Y8
G	-10	HIS	-	expression tag	UNP M5A5Y8
G	-9	SER	-	expression tag	UNP M5A5Y8
G	-8	SER	-	expression tag	UNP M5A5Y8
G	-7	GLY	-	expression tag	UNP M5A5Y8
G	-6	LEU	-	expression tag	UNP M5A5Y8
G	-5	VAL	-	expression tag	UNP M5A5Y8

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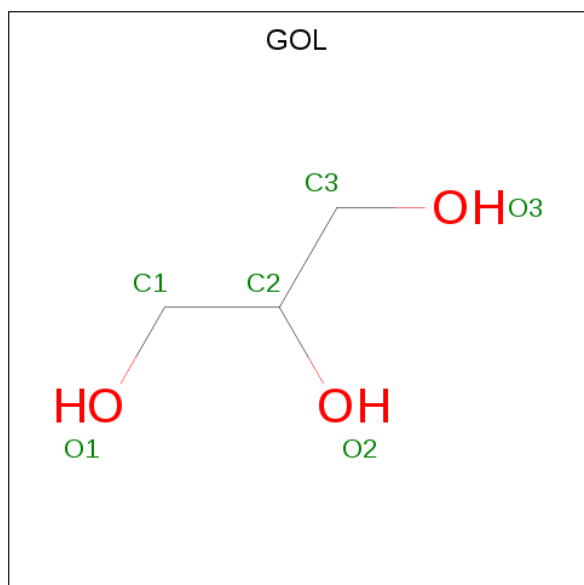
Chain	Residue	Modelled	Actual	Comment	Reference
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G	-3	ARG	-	expression tag	UNP M5A5Y8
G	-2	GLY	-	expression tag	UNP M5A5Y8
G	-1	SER	-	expression tag	UNP M5A5Y8
G	0	HIS	-	expression tag	UNP M5A5Y8
H	-19	MET	-	initiating methionine	UNP M5A5Y8
H	-18	GLY	-	expression tag	UNP M5A5Y8
H	-17	SER	-	expression tag	UNP M5A5Y8
H	-16	SER	-	expression tag	UNP M5A5Y8
H	-15	HIS	-	expression tag	UNP M5A5Y8
H	-14	HIS	-	expression tag	UNP M5A5Y8
H	-13	HIS	-	expression tag	UNP M5A5Y8
H	-12	HIS	-	expression tag	UNP M5A5Y8
H	-11	HIS	-	expression tag	UNP M5A5Y8
H	-10	HIS	-	expression tag	UNP M5A5Y8
H	-9	SER	-	expression tag	UNP M5A5Y8
H	-8	SER	-	expression tag	UNP M5A5Y8
H	-7	GLY	-	expression tag	UNP M5A5Y8
H	-6	LEU	-	expression tag	UNP M5A5Y8
H	-5	VAL	-	expression tag	UNP M5A5Y8
H	-4	PRO	-	expression tag	UNP M5A5Y8
H	-3	ARG	-	expression tag	UNP M5A5Y8
H	-2	GLY	-	expression tag	UNP M5A5Y8
H	-1	SER	-	expression tag	UNP M5A5Y8
H	0	HIS	-	expression tag	UNP M5A5Y8
I	-19	MET	-	initiating methionine	UNP M5A5Y8
I	-18	GLY	-	expression tag	UNP M5A5Y8
I	-17	SER	-	expression tag	UNP M5A5Y8
I	-16	SER	-	expression tag	UNP M5A5Y8
I	-15	HIS	-	expression tag	UNP M5A5Y8
I	-14	HIS	-	expression tag	UNP M5A5Y8
I	-13	HIS	-	expression tag	UNP M5A5Y8
I	-12	HIS	-	expression tag	UNP M5A5Y8
I	-11	HIS	-	expression tag	UNP M5A5Y8
I	-10	HIS	-	expression tag	UNP M5A5Y8
I	-9	SER	-	expression tag	UNP M5A5Y8
I	-8	SER	-	expression tag	UNP M5A5Y8
I	-7	GLY	-	expression tag	UNP M5A5Y8
I	-6	LEU	-	expression tag	UNP M5A5Y8
I	-5	VAL	-	expression tag	UNP M5A5Y8
I	-4	PRO	-	expression tag	UNP M5A5Y8
I	-3	ARG	-	expression tag	UNP M5A5Y8

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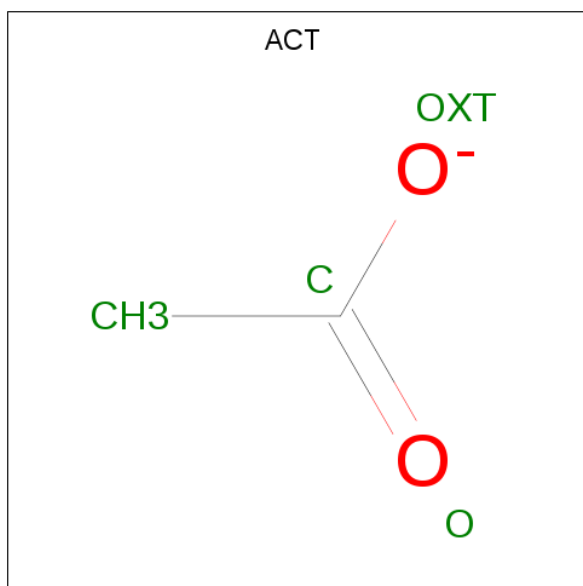
Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	expression tag	UNP M5A5Y8
I	-1	SER	-	expression tag	UNP M5A5Y8
I	0	HIS	-	expression tag	UNP M5A5Y8
J	-19	MET	-	initiating methionine	UNP M5A5Y8
J	-18	GLY	-	expression tag	UNP M5A5Y8
J	-17	SER	-	expression tag	UNP M5A5Y8
J	-16	SER	-	expression tag	UNP M5A5Y8
J	-15	HIS	-	expression tag	UNP M5A5Y8
J	-14	HIS	-	expression tag	UNP M5A5Y8
J	-13	HIS	-	expression tag	UNP M5A5Y8
J	-12	HIS	-	expression tag	UNP M5A5Y8
J	-11	HIS	-	expression tag	UNP M5A5Y8
J	-10	HIS	-	expression tag	UNP M5A5Y8
J	-9	SER	-	expression tag	UNP M5A5Y8
J	-8	SER	-	expression tag	UNP M5A5Y8
J	-7	GLY	-	expression tag	UNP M5A5Y8
J	-6	LEU	-	expression tag	UNP M5A5Y8
J	-5	VAL	-	expression tag	UNP M5A5Y8
J	-4	PRO	-	expression tag	UNP M5A5Y8
J	-3	ARG	-	expression tag	UNP M5A5Y8
J	-2	GLY	-	expression tag	UNP M5A5Y8
J	-1	SER	-	expression tag	UNP M5A5Y8
J	0	HIS	-	expression tag	UNP M5A5Y8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	172	Total	O	0	0
			172	172		
4	C	120	Total	O	0	0
			120	120		
4	D	160	Total	O	0	0
			160	160		
4	E	188	Total	O	0	0
			188	188		
4	F	188	Total	O	0	0
			188	188		
4	G	73	Total	O	0	0
			73	73		

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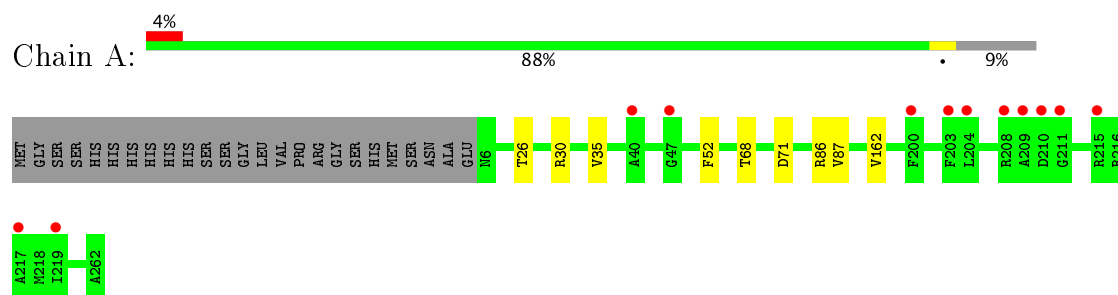
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	57	Total 57	O 57	0	0
4	I	52	Total 52	O 52	0	0
4	J	84	Total 84	O 84	0	0

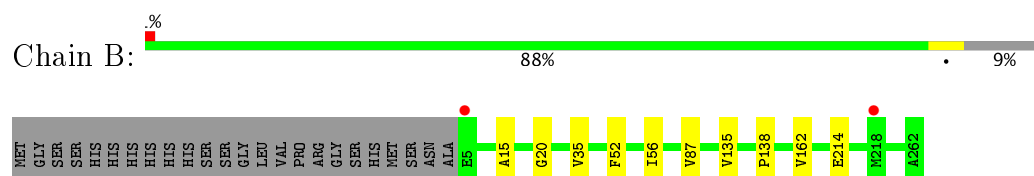
3 Residue-property plots [i](#)

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.

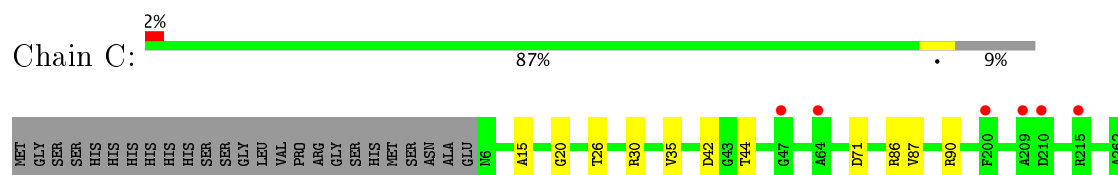
- Molecule 1: Putative oxidoreductase



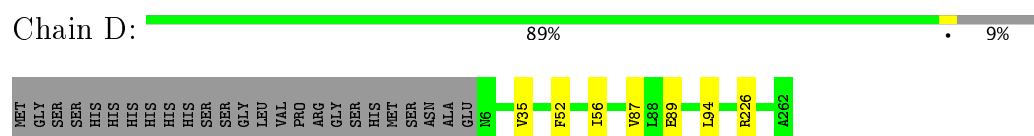
- Molecule 1: Putative oxidoreductase



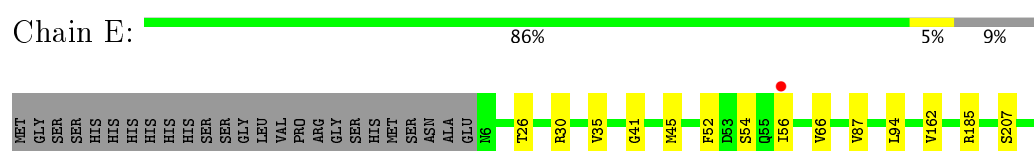
- Molecule 1: Putative oxidoreductase




- Molecule 1: Putative oxidoreductase

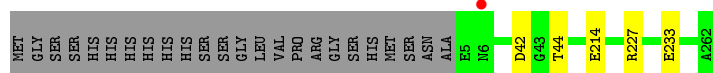


- Molecule 1: Putative oxidoreductase




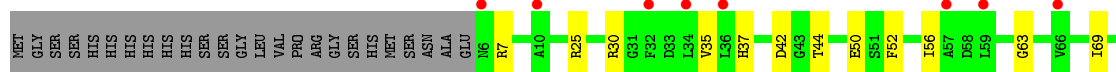
- Molecule 1: Putative oxidoreductase

Chain F:  90% 9%




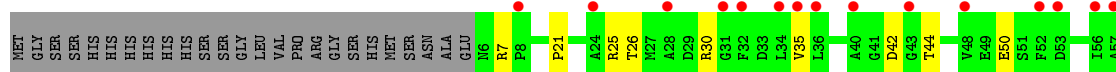
- Molecule 1: Putative oxidoreductase

Chain G:  84% 7% 9% 4%




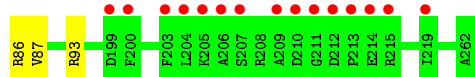
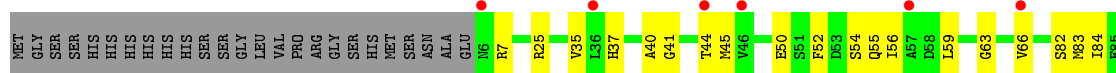
- Molecule 1: Putative oxidoreductase

Chain H:  85% 6% 9% 15%




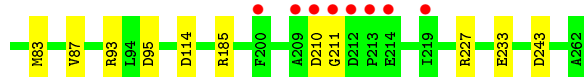
- Molecule 1: Putative oxidoreductase

Chain I:  83% 8% 9% 7%



- Molecule 1: Putative oxidoreductase

Chain J:  81% 10% 9% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	194.88Å 194.88Å 195.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.06 – 2.30 68.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.06-2.30) 100.0 (68.95-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.29Å)	Xtriage
Refinement program	PHENIX (dev_2666: ???)	Depositor
R, R_{free}	0.190 , 0.203 0.181 , 0.196	Depositor DCC
R_{free} test set	9636 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	38900	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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

5.1 Standard geometry

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

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	0.25	0/1959	0.47	0/2651
1	B	0.26	0/1953	0.47	0/2643
1	C	0.25	0/1966	0.47	0/2661
1	D	0.26	0/1946	0.46	0/2636
1	E	0.26	0/1938	0.47	0/2623
1	F	0.26	0/1963	0.48	0/2654
1	G	0.26	0/1928	0.47	0/2614
1	H	0.26	0/1913	0.47	0/2594
1	I	0.27	0/1899	0.50	0/2576
1	J	0.29	0/1914	0.47	0/2594
All	All	0.26	0/19379	0.47	0/26246

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	1913	1883	1890	5	0
1	B	1913	1880	1885	5	0
1	C	1920	1889	1895	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1906	1869	1874	5	0
1	E	1904	1874	1876	9	0
1	F	1923	1902	1907	3	0
1	G	1891	1842	1844	10	0
1	H	1879	1831	1832	12	0
1	I	1868	1815	1817	13	0
1	J	1883	1838	1838	20	0
2	A	6	8	8	0	0
3	B	8	6	6	0	0
4	A	155	0	0	0	0
4	B	172	0	0	0	1
4	C	120	0	0	0	0
4	D	160	0	0	2	1
4	E	188	0	0	0	0
4	F	188	0	0	0	0
4	G	73	0	0	1	0
4	H	57	0	0	0	0
4	I	52	0	0	0	0
4	J	84	0	0	2	0
All	All	20263	18637	18672	89	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 2.

The worst 5 of 89 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:J:7:ARG:NH1	1:J:63:GLY:O	1.64	1.31
1:J:7:ARG:HH12	1:J:63:GLY:C	1.47	1.14
1:I:7:ARG:NH1	1:I:63:GLY:O	2.01	0.93
1:A:71:ASP:OD1	1:A:86[B]:ARG:NH2	2.11	0.84
1:H:7:ARG:NH1	1:H:63:GLY:O	2.12	0.83

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)
4:B:523:HOH:O	4:D:312:HOH:O[2_655]	1.92	0.28

5.3 Torsion angles

5.3.1 Protein backbone

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	260/282 (92%)	252 (97%)	8 (3%)	0	100	100
1	B	259/282 (92%)	250 (96%)	9 (4%)	0	100	100
1	C	260/282 (92%)	251 (96%)	9 (4%)	0	100	100
1	D	258/282 (92%)	249 (96%)	9 (4%)	0	100	100
1	E	256/282 (91%)	247 (96%)	9 (4%)	0	100	100
1	F	259/282 (92%)	250 (96%)	9 (4%)	0	100	100
1	G	257/282 (91%)	248 (96%)	9 (4%)	0	100	100
1	H	256/282 (91%)	246 (96%)	10 (4%)	0	100	100
1	I	255/282 (90%)	247 (97%)	8 (3%)	0	100	100
1	J	255/282 (90%)	246 (96%)	9 (4%)	0	100	100
All	All	2575/2820 (91%)	2486 (96%)	89 (4%)	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	197/217 (91%)	197 (100%)	0	100	100
1	B	197/217 (91%)	196 (100%)	1 (0%)	91	96
1	C	197/217 (91%)	197 (100%)	0	100	100
1	D	196/217 (90%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	196/217 (90%)	194 (99%)	2 (1%)	80	90
1	F	199/217 (92%)	198 (100%)	1 (0%)	91	96
1	G	193/217 (89%)	191 (99%)	2 (1%)	80	90
1	H	189/217 (87%)	189 (100%)	0	100	100
1	I	187/217 (86%)	185 (99%)	2 (1%)	78	89
1	J	191/217 (88%)	188 (98%)	3 (2%)	68	82
All	All	1942/2170 (90%)	1931 (99%)	11 (1%)	89	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	84	ILE
1	G	103	LEU
1	J	56	ILE
1	F	214	GLU
1	I	54	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	GOL	A	301	-	5,5,5	0.91	0	5,5,5	0.94	0
3	ACT	B	301	-	1,3,3	6.01	1 (100%)	0,3,3	0.00	-
3	ACT	B	302	-	1,3,3	5.97	1 (100%)	0,3,3	0.00	-

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
2	GOL	A	301	-	-	0/4/4/4	0/0/0/0
3	ACT	B	301	-	-	0/0/0/0	0/0/0/0
3	ACT	B	302	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	ACT	CH3-C	5.97	1.56	1.48
3	B	301	ACT	CH3-C	6.01	1.56	1.48

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 ⓘ

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	257/282 (91%)	0.31	12 (4%) 32 39	35, 51, 107, 153	0
1	B	258/282 (91%)	0.23	2 (0%) 86 89	34, 48, 78, 127	0
1	C	257/282 (91%)	0.26	6 (2%) 61 67	37, 56, 110, 178	0
1	D	257/282 (91%)	0.05	0 100 100	35, 53, 81, 125	0
1	E	257/282 (91%)	0.04	1 (0%) 92 95	32, 45, 81, 104	0
1	F	258/282 (91%)	-0.04	1 (0%) 92 95	33, 45, 80, 115	0
1	G	257/282 (91%)	0.25	11 (4%) 36 43	45, 72, 119, 175	0
1	H	257/282 (91%)	0.81	41 (15%) 2 3	56, 77, 117, 190	0
1	I	257/282 (91%)	0.37	21 (8%) 12 17	55, 74, 117, 172	0
1	J	257/282 (91%)	0.37	19 (7%) 15 21	46, 70, 124, 158	0
All	All	2572/2820 (91%)	0.26	114 (4%) 35 42	32, 59, 110, 190	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	66	VAL	6.9
1	I	211	GLY	6.5
1	A	209	ALA	6.4
1	I	209	ALA	6.0
1	H	67	LEU	5.4

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 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. 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(\AA^2)	Q<0.9
2	GOL	A	301	6/6	0.88	0.13	-1.33	78,93,94,94	0
3	ACT	B	301	4/4	0.86	0.17	-	88,90,108,108	0
3	ACT	B	302	4/4	0.90	0.57	-	89,91,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.