wwPDB X-ray Structure Validation Summary Report (i)

Jun 22, 2024 – 09:03 PM EDT

PDB ID	:	6D1O
Title	:	FT_5 dioxygenase apoenzyme
Authors	:	Rydel, T.J.; Halls, C.E.
Deposited on	:	2018-04-12
Resolution	:	2.70 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:

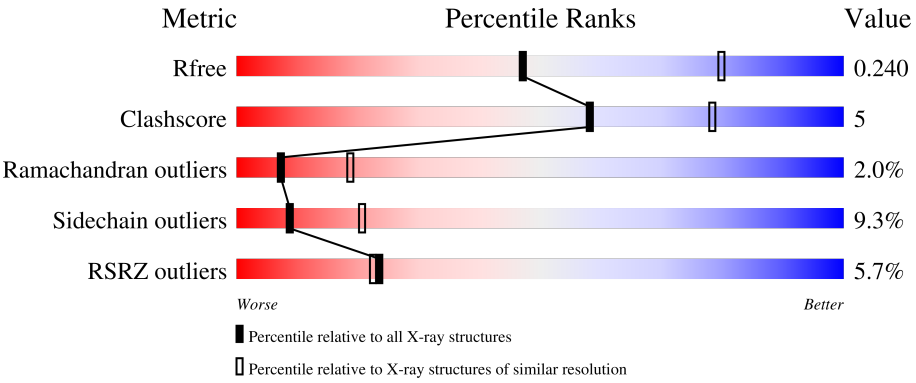
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	301	4% 70% 15% •• 12%
1	B	301	3% 68% 17% •• 13%
1	C	301	8% 72% 13% •• 12%
1	D	301	7% 69% 15% • • 12%
1	E	301	5% 69% 14% • • 12%

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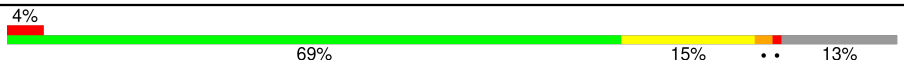
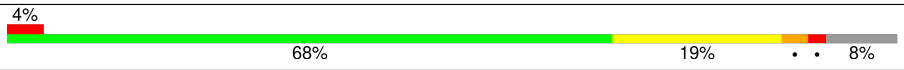
Mol	Chain	Length	Quality of chain
1	F	301	
1	G	301	
1	H	301	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17210 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 (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2105	1343	358	395	9			
1	B	263	Total	C	N	O	S	0	0	0
			2094	1337	354	394	9			
1	C	266	Total	C	N	O	S	0	0	0
			2125	1354	364	398	9			
1	D	265	Total	C	N	O	S	0	0	0
			2117	1349	363	397	8			
1	E	266	Total	C	N	O	S	0	0	0
			2120	1352	363	397	8			
1	F	262	Total	C	N	O	S	0	0	0
			2092	1336	358	390	8			
1	G	275	Total	C	N	O	S	0	0	0
			2190	1391	379	412	8			
1	H	276	Total	C	N	O	S	0	0	0
			2194	1393	378	415	8			

There are 272 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	GLU	ASP	conflict	UNP Q8KSC8
A	109	ASN	ASP	conflict	UNP Q8KSC8
A	127	TYR	ARG	conflict	UNP Q8KSC8
A	129	LYS	ILE	conflict	UNP Q8KSC8
A	130	GLU	ASP	conflict	UNP Q8KSC8
A	131	ILE	VAL	conflict	UNP Q8KSC8
A	133	PRO	GLU	conflict	UNP Q8KSC8
A	134	TYR	HIS	conflict	UNP Q8KSC8
A	139	LEU	GLY	conflict	UNP Q8KSC8
A	141	THR	LEU	conflict	UNP Q8KSC8
A	209	GLU	GLY	conflict	UNP Q8KSC8
A	210	THR	SER	conflict	UNP Q8KSC8
A	229	SER	THR	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLU	ASP	conflict	UNP Q8KSC8
A	231	LYS	ALA	conflict	UNP Q8KSC8
A	234	GLU	LYS	conflict	UNP Q8KSC8
A	238	SER	GLN	conflict	UNP Q8KSC8
A	241	PHE	TYR	conflict	UNP Q8KSC8
A	242	ALA	GLU	conflict	UNP Q8KSC8
A	246	LYS	ARG	conflict	UNP Q8KSC8
A	247	PRO	PHE	conflict	UNP Q8KSC8
A	248	GLU	ASP	conflict	UNP Q8KSC8
A	256	GLN	LYS	conflict	UNP Q8KSC8
A	257	GLU	LYS	conflict	UNP Q8KSC8
A	258	GLY	ASP	conflict	UNP Q8KSC8
A	259	ASP	GLN	conflict	UNP Q8KSC8
A	269	GLN	MET	conflict	UNP Q8KSC8
A	271	TYR	ARG	conflict	UNP Q8KSC8
A	296	HIS	-	expression tag	UNP Q8KSC8
A	297	HIS	-	expression tag	UNP Q8KSC8
A	298	HIS	-	expression tag	UNP Q8KSC8
A	299	HIS	-	expression tag	UNP Q8KSC8
A	300	HIS	-	expression tag	UNP Q8KSC8
A	301	HIS	-	expression tag	UNP Q8KSC8
B	108	GLU	ASP	conflict	UNP Q8KSC8
B	109	ASN	ASP	conflict	UNP Q8KSC8
B	127	TYR	ARG	conflict	UNP Q8KSC8
B	129	LYS	ILE	conflict	UNP Q8KSC8
B	130	GLU	ASP	conflict	UNP Q8KSC8
B	131	ILE	VAL	conflict	UNP Q8KSC8
B	133	PRO	GLU	conflict	UNP Q8KSC8
B	134	TYR	HIS	conflict	UNP Q8KSC8
B	139	LEU	GLY	conflict	UNP Q8KSC8
B	141	THR	LEU	conflict	UNP Q8KSC8
B	209	GLU	GLY	conflict	UNP Q8KSC8
B	210	THR	SER	conflict	UNP Q8KSC8
B	229	SER	THR	conflict	UNP Q8KSC8
B	230	GLU	ASP	conflict	UNP Q8KSC8
B	231	LYS	ALA	conflict	UNP Q8KSC8
B	234	GLU	LYS	conflict	UNP Q8KSC8
B	238	SER	GLN	conflict	UNP Q8KSC8
B	241	PHE	TYR	conflict	UNP Q8KSC8
B	242	ALA	GLU	conflict	UNP Q8KSC8
B	246	LYS	ARG	conflict	UNP Q8KSC8
B	247	PRO	PHE	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	248	GLU	ASP	conflict	UNP Q8KSC8
B	256	GLN	LYS	conflict	UNP Q8KSC8
B	257	GLU	LYS	conflict	UNP Q8KSC8
B	258	GLY	ASP	conflict	UNP Q8KSC8
B	259	ASP	GLN	conflict	UNP Q8KSC8
B	269	GLN	MET	conflict	UNP Q8KSC8
B	271	TYR	ARG	conflict	UNP Q8KSC8
B	296	HIS	-	expression tag	UNP Q8KSC8
B	297	HIS	-	expression tag	UNP Q8KSC8
B	298	HIS	-	expression tag	UNP Q8KSC8
B	299	HIS	-	expression tag	UNP Q8KSC8
B	300	HIS	-	expression tag	UNP Q8KSC8
B	301	HIS	-	expression tag	UNP Q8KSC8
C	108	GLU	ASP	conflict	UNP Q8KSC8
C	109	ASN	ASP	conflict	UNP Q8KSC8
C	127	TYR	ARG	conflict	UNP Q8KSC8
C	129	LYS	ILE	conflict	UNP Q8KSC8
C	130	GLU	ASP	conflict	UNP Q8KSC8
C	131	ILE	VAL	conflict	UNP Q8KSC8
C	133	PRO	GLU	conflict	UNP Q8KSC8
C	134	TYR	HIS	conflict	UNP Q8KSC8
C	139	LEU	GLY	conflict	UNP Q8KSC8
C	141	THR	LEU	conflict	UNP Q8KSC8
C	209	GLU	GLY	conflict	UNP Q8KSC8
C	210	THR	SER	conflict	UNP Q8KSC8
C	229	SER	THR	conflict	UNP Q8KSC8
C	230	GLU	ASP	conflict	UNP Q8KSC8
C	231	LYS	ALA	conflict	UNP Q8KSC8
C	234	GLU	LYS	conflict	UNP Q8KSC8
C	238	SER	GLN	conflict	UNP Q8KSC8
C	241	PHE	TYR	conflict	UNP Q8KSC8
C	242	ALA	GLU	conflict	UNP Q8KSC8
C	246	LYS	ARG	conflict	UNP Q8KSC8
C	247	PRO	PHE	conflict	UNP Q8KSC8
C	248	GLU	ASP	conflict	UNP Q8KSC8
C	256	GLN	LYS	conflict	UNP Q8KSC8
C	257	GLU	LYS	conflict	UNP Q8KSC8
C	258	GLY	ASP	conflict	UNP Q8KSC8
C	259	ASP	GLN	conflict	UNP Q8KSC8
C	269	GLN	MET	conflict	UNP Q8KSC8
C	271	TYR	ARG	conflict	UNP Q8KSC8
C	296	HIS	-	expression tag	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	297	HIS	-	expression tag	UNP Q8KSC8
C	298	HIS	-	expression tag	UNP Q8KSC8
C	299	HIS	-	expression tag	UNP Q8KSC8
C	300	HIS	-	expression tag	UNP Q8KSC8
C	301	HIS	-	expression tag	UNP Q8KSC8
D	108	GLU	ASP	conflict	UNP Q8KSC8
D	109	ASN	ASP	conflict	UNP Q8KSC8
D	127	TYR	ARG	conflict	UNP Q8KSC8
D	129	LYS	ILE	conflict	UNP Q8KSC8
D	130	GLU	ASP	conflict	UNP Q8KSC8
D	131	ILE	VAL	conflict	UNP Q8KSC8
D	133	PRO	GLU	conflict	UNP Q8KSC8
D	134	TYR	HIS	conflict	UNP Q8KSC8
D	139	LEU	GLY	conflict	UNP Q8KSC8
D	141	THR	LEU	conflict	UNP Q8KSC8
D	209	GLU	GLY	conflict	UNP Q8KSC8
D	210	THR	SER	conflict	UNP Q8KSC8
D	229	SER	THR	conflict	UNP Q8KSC8
D	230	GLU	ASP	conflict	UNP Q8KSC8
D	231	LYS	ALA	conflict	UNP Q8KSC8
D	234	GLU	LYS	conflict	UNP Q8KSC8
D	238	SER	GLN	conflict	UNP Q8KSC8
D	241	PHE	TYR	conflict	UNP Q8KSC8
D	242	ALA	GLU	conflict	UNP Q8KSC8
D	246	LYS	ARG	conflict	UNP Q8KSC8
D	247	PRO	PHE	conflict	UNP Q8KSC8
D	248	GLU	ASP	conflict	UNP Q8KSC8
D	256	GLN	LYS	conflict	UNP Q8KSC8
D	257	GLU	LYS	conflict	UNP Q8KSC8
D	258	GLY	ASP	conflict	UNP Q8KSC8
D	259	ASP	GLN	conflict	UNP Q8KSC8
D	269	GLN	MET	conflict	UNP Q8KSC8
D	271	TYR	ARG	conflict	UNP Q8KSC8
D	296	HIS	-	expression tag	UNP Q8KSC8
D	297	HIS	-	expression tag	UNP Q8KSC8
D	298	HIS	-	expression tag	UNP Q8KSC8
D	299	HIS	-	expression tag	UNP Q8KSC8
D	300	HIS	-	expression tag	UNP Q8KSC8
D	301	HIS	-	expression tag	UNP Q8KSC8
E	108	GLU	ASP	conflict	UNP Q8KSC8
E	109	ASN	ASP	conflict	UNP Q8KSC8
E	127	TYR	ARG	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	129	LYS	ILE	conflict	UNP Q8KSC8
E	130	GLU	ASP	conflict	UNP Q8KSC8
E	131	ILE	VAL	conflict	UNP Q8KSC8
E	133	PRO	GLU	conflict	UNP Q8KSC8
E	134	TYR	HIS	conflict	UNP Q8KSC8
E	139	LEU	GLY	conflict	UNP Q8KSC8
E	141	THR	LEU	conflict	UNP Q8KSC8
E	209	GLU	GLY	conflict	UNP Q8KSC8
E	210	THR	SER	conflict	UNP Q8KSC8
E	229	SER	THR	conflict	UNP Q8KSC8
E	230	GLU	ASP	conflict	UNP Q8KSC8
E	231	LYS	ALA	conflict	UNP Q8KSC8
E	234	GLU	LYS	conflict	UNP Q8KSC8
E	238	SER	GLN	conflict	UNP Q8KSC8
E	241	PHE	TYR	conflict	UNP Q8KSC8
E	242	ALA	GLU	conflict	UNP Q8KSC8
E	246	LYS	ARG	conflict	UNP Q8KSC8
E	247	PRO	PHE	conflict	UNP Q8KSC8
E	248	GLU	ASP	conflict	UNP Q8KSC8
E	256	GLN	LYS	conflict	UNP Q8KSC8
E	257	GLU	LYS	conflict	UNP Q8KSC8
E	258	GLY	ASP	conflict	UNP Q8KSC8
E	259	ASP	GLN	conflict	UNP Q8KSC8
E	269	GLN	MET	conflict	UNP Q8KSC8
E	271	TYR	ARG	conflict	UNP Q8KSC8
E	296	HIS	-	expression tag	UNP Q8KSC8
E	297	HIS	-	expression tag	UNP Q8KSC8
E	298	HIS	-	expression tag	UNP Q8KSC8
E	299	HIS	-	expression tag	UNP Q8KSC8
E	300	HIS	-	expression tag	UNP Q8KSC8
E	301	HIS	-	expression tag	UNP Q8KSC8
F	108	GLU	ASP	conflict	UNP Q8KSC8
F	109	ASN	ASP	conflict	UNP Q8KSC8
F	127	TYR	ARG	conflict	UNP Q8KSC8
F	129	LYS	ILE	conflict	UNP Q8KSC8
F	130	GLU	ASP	conflict	UNP Q8KSC8
F	131	ILE	VAL	conflict	UNP Q8KSC8
F	133	PRO	GLU	conflict	UNP Q8KSC8
F	134	TYR	HIS	conflict	UNP Q8KSC8
F	139	LEU	GLY	conflict	UNP Q8KSC8
F	141	THR	LEU	conflict	UNP Q8KSC8
F	209	GLU	GLY	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	210	THR	SER	conflict	UNP Q8KSC8
F	229	SER	THR	conflict	UNP Q8KSC8
F	230	GLU	ASP	conflict	UNP Q8KSC8
F	231	LYS	ALA	conflict	UNP Q8KSC8
F	234	GLU	LYS	conflict	UNP Q8KSC8
F	238	SER	GLN	conflict	UNP Q8KSC8
F	241	PHE	TYR	conflict	UNP Q8KSC8
F	242	ALA	GLU	conflict	UNP Q8KSC8
F	246	LYS	ARG	conflict	UNP Q8KSC8
F	247	PRO	PHE	conflict	UNP Q8KSC8
F	248	GLU	ASP	conflict	UNP Q8KSC8
F	256	GLN	LYS	conflict	UNP Q8KSC8
F	257	GLU	LYS	conflict	UNP Q8KSC8
F	258	GLY	ASP	conflict	UNP Q8KSC8
F	259	ASP	GLN	conflict	UNP Q8KSC8
F	269	GLN	MET	conflict	UNP Q8KSC8
F	271	TYR	ARG	conflict	UNP Q8KSC8
F	296	HIS	-	expression tag	UNP Q8KSC8
F	297	HIS	-	expression tag	UNP Q8KSC8
F	298	HIS	-	expression tag	UNP Q8KSC8
F	299	HIS	-	expression tag	UNP Q8KSC8
F	300	HIS	-	expression tag	UNP Q8KSC8
F	301	HIS	-	expression tag	UNP Q8KSC8
G	108	GLU	ASP	conflict	UNP Q8KSC8
G	109	ASN	ASP	conflict	UNP Q8KSC8
G	127	TYR	ARG	conflict	UNP Q8KSC8
G	129	LYS	ILE	conflict	UNP Q8KSC8
G	130	GLU	ASP	conflict	UNP Q8KSC8
G	131	ILE	VAL	conflict	UNP Q8KSC8
G	133	PRO	GLU	conflict	UNP Q8KSC8
G	134	TYR	HIS	conflict	UNP Q8KSC8
G	139	LEU	GLY	conflict	UNP Q8KSC8
G	141	THR	LEU	conflict	UNP Q8KSC8
G	209	GLU	GLY	conflict	UNP Q8KSC8
G	210	THR	SER	conflict	UNP Q8KSC8
G	229	SER	THR	conflict	UNP Q8KSC8
G	230	GLU	ASP	conflict	UNP Q8KSC8
G	231	LYS	ALA	conflict	UNP Q8KSC8
G	234	GLU	LYS	conflict	UNP Q8KSC8
G	238	SER	GLN	conflict	UNP Q8KSC8
G	241	PHE	TYR	conflict	UNP Q8KSC8
G	242	ALA	GLU	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	246	LYS	ARG	conflict	UNP Q8KSC8
G	247	PRO	PHE	conflict	UNP Q8KSC8
G	248	GLU	ASP	conflict	UNP Q8KSC8
G	256	GLN	LYS	conflict	UNP Q8KSC8
G	257	GLU	LYS	conflict	UNP Q8KSC8
G	258	GLY	ASP	conflict	UNP Q8KSC8
G	259	ASP	GLN	conflict	UNP Q8KSC8
G	269	GLN	MET	conflict	UNP Q8KSC8
G	271	TYR	ARG	conflict	UNP Q8KSC8
G	296	HIS	-	expression tag	UNP Q8KSC8
G	297	HIS	-	expression tag	UNP Q8KSC8
G	298	HIS	-	expression tag	UNP Q8KSC8
G	299	HIS	-	expression tag	UNP Q8KSC8
G	300	HIS	-	expression tag	UNP Q8KSC8
G	301	HIS	-	expression tag	UNP Q8KSC8
H	108	GLU	ASP	conflict	UNP Q8KSC8
H	109	ASN	ASP	conflict	UNP Q8KSC8
H	127	TYR	ARG	conflict	UNP Q8KSC8
H	129	LYS	ILE	conflict	UNP Q8KSC8
H	130	GLU	ASP	conflict	UNP Q8KSC8
H	131	ILE	VAL	conflict	UNP Q8KSC8
H	133	PRO	GLU	conflict	UNP Q8KSC8
H	134	TYR	HIS	conflict	UNP Q8KSC8
H	139	LEU	GLY	conflict	UNP Q8KSC8
H	141	THR	LEU	conflict	UNP Q8KSC8
H	209	GLU	GLY	conflict	UNP Q8KSC8
H	210	THR	SER	conflict	UNP Q8KSC8
H	229	SER	THR	conflict	UNP Q8KSC8
H	230	GLU	ASP	conflict	UNP Q8KSC8
H	231	LYS	ALA	conflict	UNP Q8KSC8
H	234	GLU	LYS	conflict	UNP Q8KSC8
H	238	SER	GLN	conflict	UNP Q8KSC8
H	241	PHE	TYR	conflict	UNP Q8KSC8
H	242	ALA	GLU	conflict	UNP Q8KSC8
H	246	LYS	ARG	conflict	UNP Q8KSC8
H	247	PRO	PHE	conflict	UNP Q8KSC8
H	248	GLU	ASP	conflict	UNP Q8KSC8
H	256	GLN	LYS	conflict	UNP Q8KSC8
H	257	GLU	LYS	conflict	UNP Q8KSC8
H	258	GLY	ASP	conflict	UNP Q8KSC8
H	259	ASP	GLN	conflict	UNP Q8KSC8
H	269	GLN	MET	conflict	UNP Q8KSC8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	271	TYR	ARG	conflict	UNP Q8KSC8
H	296	HIS	-	expression tag	UNP Q8KSC8
H	297	HIS	-	expression tag	UNP Q8KSC8
H	298	HIS	-	expression tag	UNP Q8KSC8
H	299	HIS	-	expression tag	UNP Q8KSC8
H	300	HIS	-	expression tag	UNP Q8KSC8
H	301	HIS	-	expression tag	UNP Q8KSC8

- Molecule 2 is water.

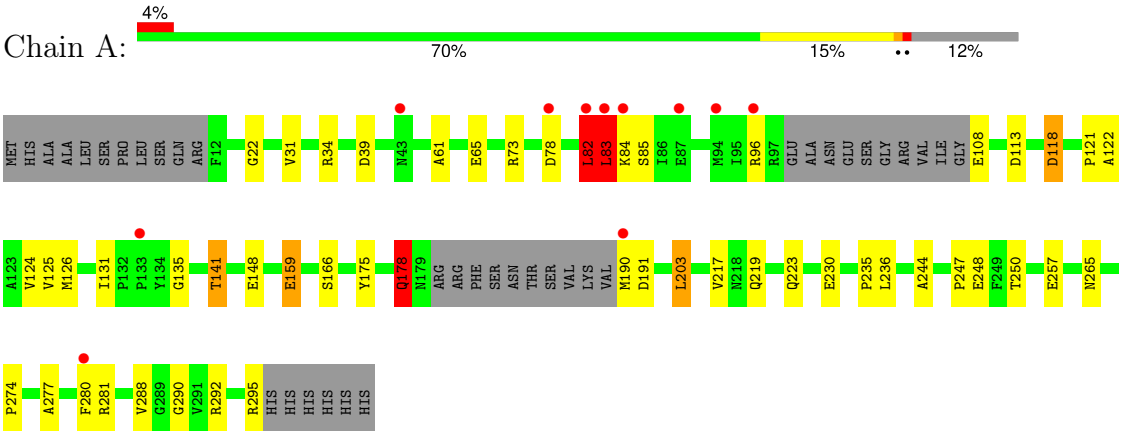
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	19	Total O 19 19	0	0
2	B	23	Total O 23 23	0	0
2	C	17	Total O 17 17	0	0
2	D	14	Total O 14 14	0	0
2	E	35	Total O 35 35	0	0
2	F	34	Total O 34 34	0	0
2	G	17	Total O 17 17	0	0
2	H	14	Total O 14 14	0	0

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.

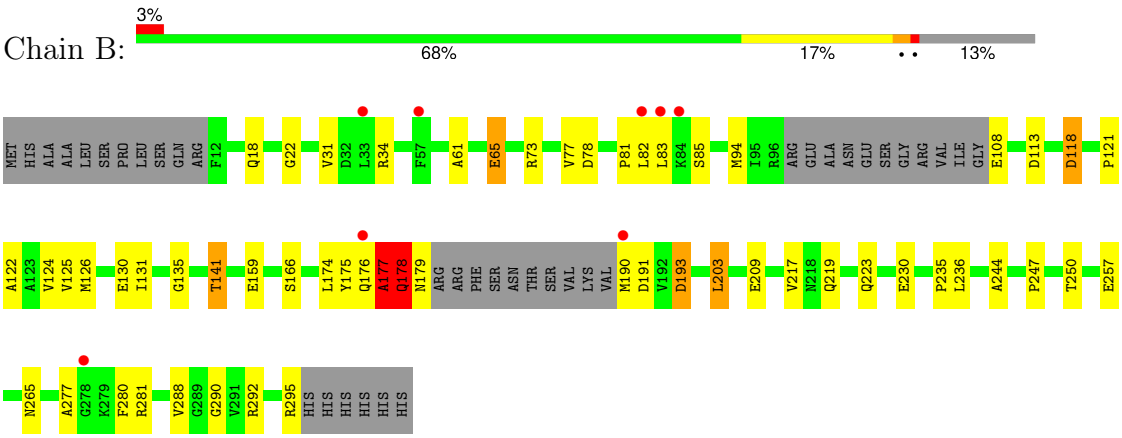
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain A:



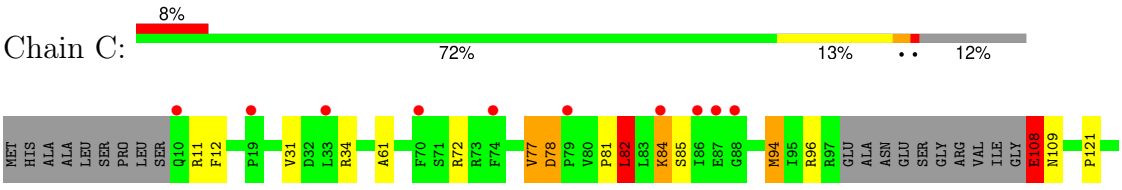
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

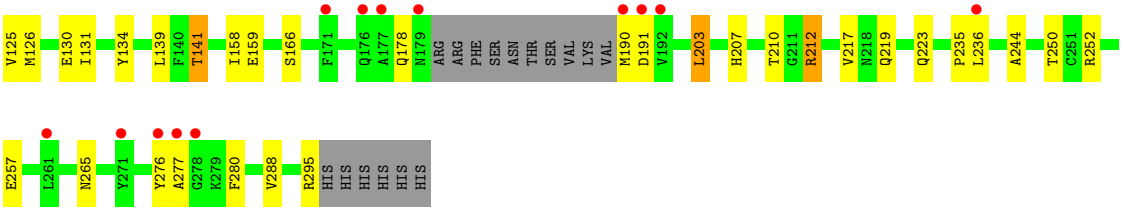
Chain B:



• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

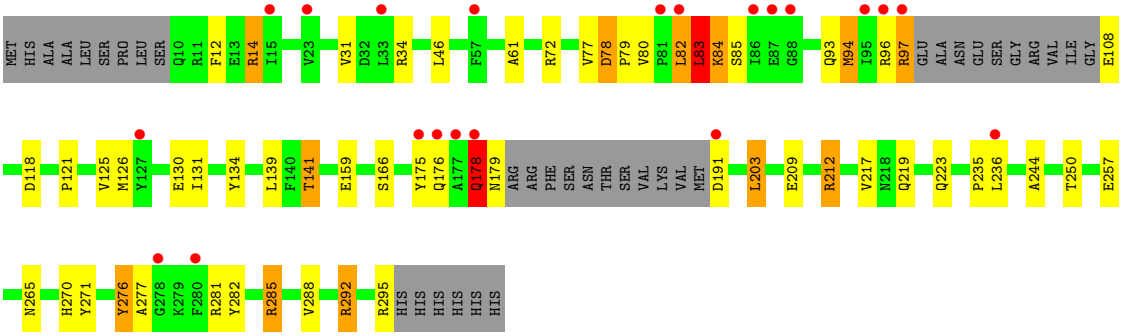
Chain C:





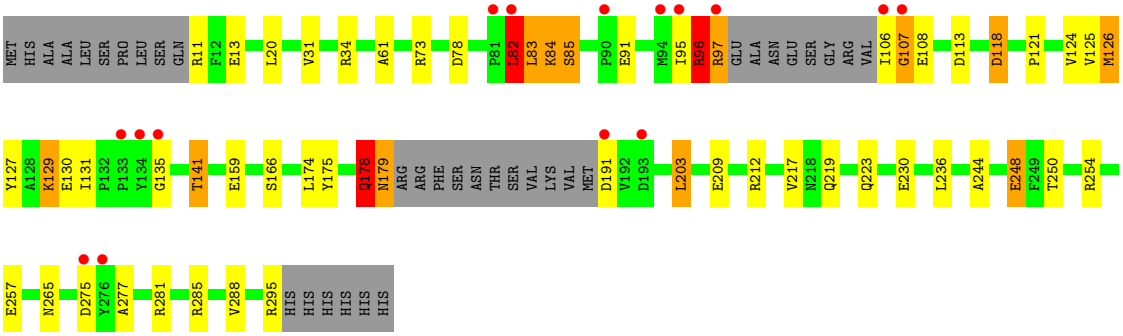
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain D:



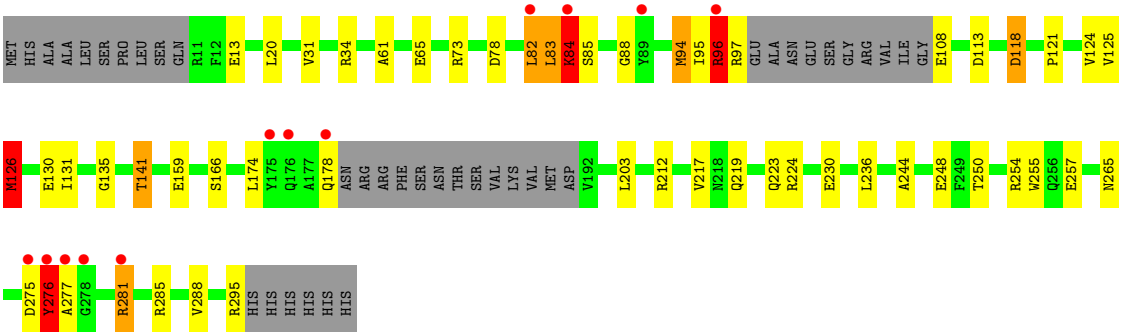
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain E:



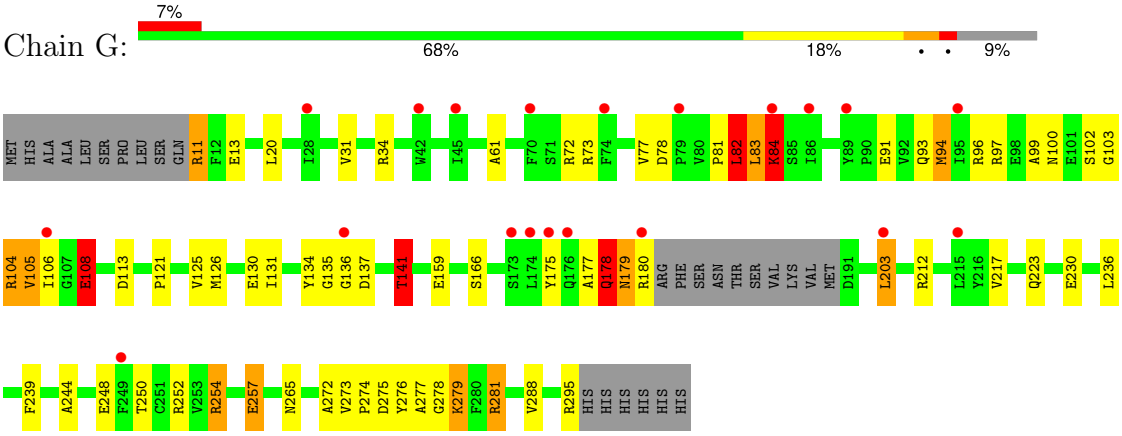
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain F:



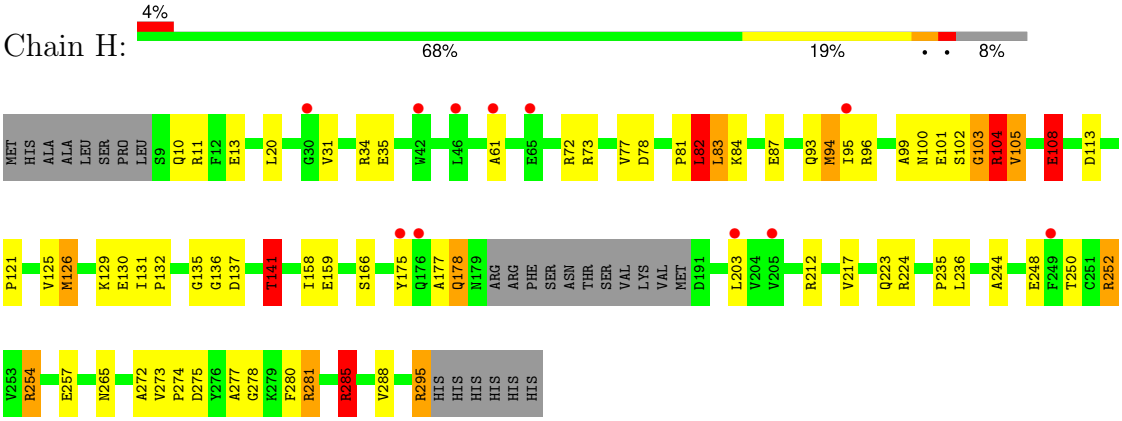
• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

Chain G:



• Molecule 1: (R)-phenoxypropionate/alpha-ketoglutarate-dioxygenase

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	70.46Å 200.33Å 98.31Å 90.00° 110.95° 90.00°	Depositor
Resolution (Å)	46.19 – 2.70 45.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.19-2.70) 97.3 (45.90-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.241 0.213 , 0.240	Depositor DCC
R_{free} test set	3438 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	1.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.460 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17210	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	1.06	5/2162 (0.2%)	1.18	18/2949 (0.6%)
1	B	1.07	6/2151 (0.3%)	1.15	17/2935 (0.6%)
1	C	0.90	3/2182 (0.1%)	1.10	16/2975 (0.5%)
1	D	0.94	4/2174 (0.2%)	1.18	21/2965 (0.7%)
1	E	1.10	9/2177 (0.4%)	1.21	18/2969 (0.6%)
1	F	1.02	4/2149 (0.2%)	1.20	24/2931 (0.8%)
1	G	1.03	8/2248 (0.4%)	1.26	26/3065 (0.8%)
1	H	1.02	4/2252 (0.2%)	1.25	27/3071 (0.9%)
All	All	1.02	43/17495 (0.2%)	1.19	167/23860 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	2
All	All	0	8

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	GLU	CD-OE2	12.10	1.39	1.25
1	A	159	GLU	CG-CD	10.35	1.67	1.51
1	E	159	GLU	CD-OE1	10.21	1.36	1.25
1	A	78	ASP	CB-CG	9.98	1.72	1.51
1	E	159	GLU	CD-OE2	9.84	1.36	1.25

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	82	LEU	CA-CB-CG	15.11	150.05	115.30
1	F	82	LEU	CA-CB-CG	15.11	150.05	115.30
1	H	82	LEU	CA-CB-CG	14.56	148.79	115.30
1	E	82	LEU	CA-CB-CG	13.11	145.44	115.30
1	G	137	ASP	CB-CG-OD2	-12.77	106.80	118.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	77	VAL	Peptide
1	C	77	VAL	Peptide
1	E	107	GLY	Peptide
1	F	96	ARG	Peptide
1	G	81	PRO	Peptide

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	2105	0	2030	15	0
1	B	2094	0	2017	15	0
1	C	2125	0	2051	20	0
1	D	2117	0	2042	29	0
1	E	2120	0	2048	22	0
1	F	2092	0	2024	17	0
1	G	2190	0	2115	31	0
1	H	2194	0	2115	42	0
2	A	19	0	0	1	0
2	B	23	0	0	1	0
2	C	17	0	0	1	0
2	D	14	0	0	1	0
2	E	35	0	0	1	0
2	F	34	0	0	2	0
2	G	17	0	0	3	0
2	H	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17210	0	16442	159	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 5.

The worst 5 of 159 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:D:46:LEU:HD23	1:H:101:GLU:HG3	1.20	1.14
1:D:212:ARG:HG2	1:H:280:PHE:CD2	1.95	1.02
1:D:80:VAL:O	1:D:83:LEU:HB3	1.66	0.93
1:G:99:ALA:HB2	1:G:278:GLY:HA3	1.50	0.91
1:A:274:PRO:HB2	1:H:87:GLU:OE2	1.72	0.90

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	258/301 (86%)	246 (95%)	8 (3%)	4 (2%)	9 24
1	B	257/301 (85%)	245 (95%)	7 (3%)	5 (2%)	8 20
1	C	260/301 (86%)	248 (95%)	7 (3%)	5 (2%)	8 20
1	D	259/301 (86%)	246 (95%)	9 (4%)	4 (2%)	10 26
1	E	260/301 (86%)	246 (95%)	9 (4%)	5 (2%)	8 20
1	F	256/301 (85%)	240 (94%)	11 (4%)	5 (2%)	7 19
1	G	271/301 (90%)	254 (94%)	9 (3%)	8 (3%)	4 10
1	H	272/301 (90%)	254 (93%)	12 (4%)	6 (2%)	6 17
All	All	2093/2408 (87%)	1979 (95%)	72 (3%)	42 (2%)	7 19

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	277	ALA
1	B	177	ALA
1	B	277	ALA
1	C	178	GLN

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	227/259 (88%)	204 (90%)	23 (10%)	7 17
1	B	226/259 (87%)	204 (90%)	22 (10%)	8 19
1	C	229/259 (88%)	211 (92%)	18 (8%)	12 28
1	D	228/259 (88%)	205 (90%)	23 (10%)	7 17
1	E	228/259 (88%)	206 (90%)	22 (10%)	8 19
1	F	225/259 (87%)	205 (91%)	20 (9%)	9 22
1	G	235/259 (91%)	213 (91%)	22 (9%)	8 20
1	H	236/259 (91%)	216 (92%)	20 (8%)	10 24
All	All	1834/2072 (88%)	1664 (91%)	170 (9%)	9 21

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	125	VAL
1	G	203	LEU
1	F	159	GLU
1	G	31	VAL
1	H	10	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	179	ASN
1	H	179	ASN
1	H	269	GLN
1	H	109	ASN
1	D	269	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	264/301 (87%)	0.21	11 (4%)	36	35	48, 62, 115, 139	0
1	B	263/301 (87%)	0.19	8 (3%)	50	51	48, 63, 110, 142	0
1	C	266/301 (88%)	0.53	23 (8%)	10	8	52, 79, 134, 185	0
1	D	265/301 (88%)	0.47	21 (7%)	12	10	52, 79, 135, 175	0
1	E	266/301 (88%)	0.21	15 (5%)	24	23	32, 49, 124, 155	0
1	F	262/301 (87%)	0.14	12 (4%)	32	31	31, 50, 112, 161	0
1	G	275/301 (91%)	0.40	20 (7%)	15	13	43, 77, 122, 157	0
1	H	276/301 (91%)	0.28	11 (3%)	38	37	42, 77, 120, 159	0
All	All	2137/2408 (88%)	0.30	121 (5%)	23	22	31, 68, 125, 185	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	106	ILE	6.9
1	C	190	MET	6.2
1	D	278	GLY	6.0
1	E	275	ASP	6.0
1	C	191	ASP	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.