Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2020 – 09:32 PM BST

PDB ID	:	5KWF
Title	:	Joint X-ray Neutron Structure of Cholesterol Oxidase
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Deposited on	:	2016-07-18
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references (i)) were used in the production of this report:

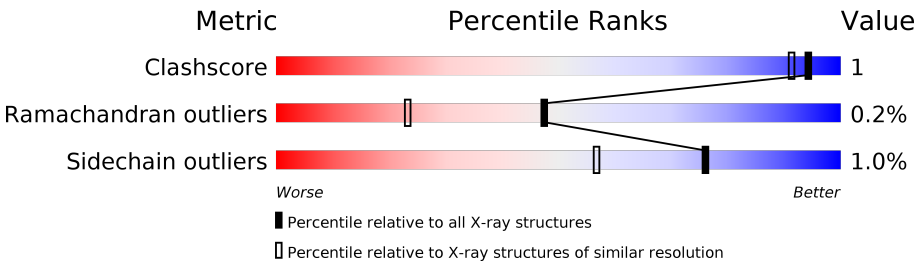
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	510	92% 6% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8991 atoms, of which 3785 are hydrogens and 1061 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.

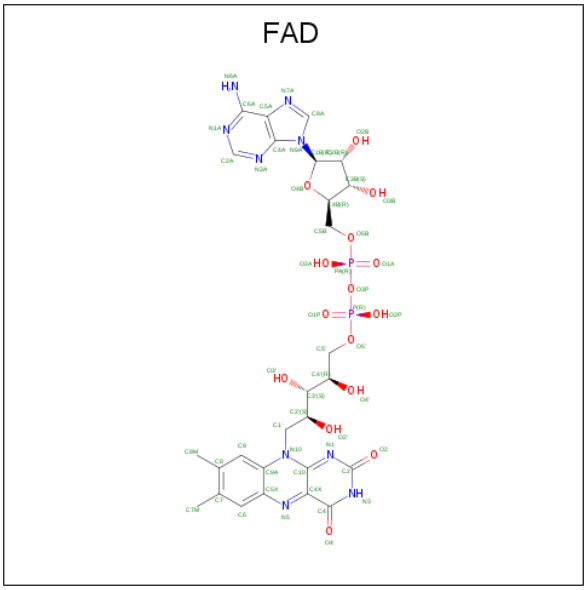
- Molecule 1 is a protein called Cholesterol oxidase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	499	8459	2424	871	3754	670	725	15	297	474	1

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	510	HIS	-	expression tag	UNP P12676
A	511	HIS	-	expression tag	UNP P12676
A	512	HIS	-	expression tag	UNP P12676
A	513	HIS	-	expression tag	UNP P12676
A	514	HIS	-	expression tag	UNP P12676
A	515	HIS	-	expression tag	UNP P12676

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	D	H	N	O	P		
2	A	1	92	27	8	31	9	15	2	4	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
3	A	258	440	182	258	5	0

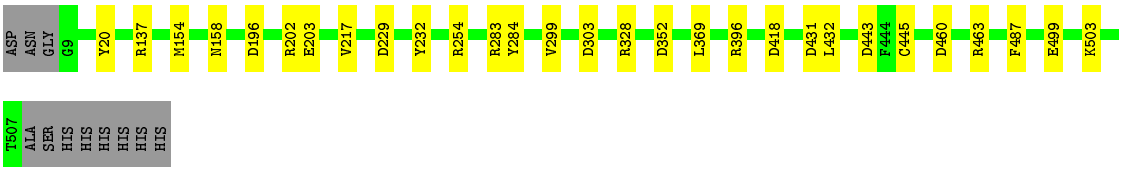
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: Cholesterol oxidase

Chain A:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.60Å 74.08Å 63.83Å 90.00° 105.21° 90.00°	Depositor
Resolution (Å)	25.26 – 1.50	Depositor
% Data completeness (in resolution range)	91.0 (25.26-1.50)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	0.26	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190 , 0.220	Depositor
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.100	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8991	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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 (i)

5.1 Standard geometry (i)

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

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	1.10	12/7658 (0.2%)	1.09	46/10404 (0.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499[A]	GLU	CD-OE2	-6.83	1.18	1.25
1	A	499[B]	GLU	CD-OE2	-6.83	1.18	1.25
1	A	445[A]	CYS	CB-SG	-6.55	1.71	1.82
1	A	445[B]	CYS	CB-SG	-6.55	1.71	1.82
1	A	284[A]	TYR	CE1-CZ	-6.20	1.30	1.38
1	A	284[B]	TYR	CE1-CZ	-6.20	1.30	1.38
1	A	299[A]	VAL	CB-CG1	-5.54	1.41	1.52
1	A	299[B]	VAL	CB-CG1	-5.54	1.41	1.52
1	A	20[A]	TYR	CD2-CE2	-5.16	1.31	1.39
1	A	20[B]	TYR	CD2-CE2	-5.16	1.31	1.39
1	A	203[A]	GLU	CG-CD	5.10	1.59	1.51
1	A	203[B]	GLU	CG-CD	5.10	1.59	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254[A]	ARG	NE-CZ-NH2	-14.09	113.26	120.30
1	A	254[B]	ARG	NE-CZ-NH2	-14.09	113.26	120.30
1	A	328[A]	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	A	328[B]	ARG	NE-CZ-NH1	9.29	124.95	120.30
1	A	137[A]	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	A	137[B]	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	A	137[A]	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	137[B]	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	254[A]	ARG	NE-CZ-NH1	6.94	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254[B]	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	232[A]	TYR	CB-CG-CD2	6.93	125.16	121.00
1	A	232[B]	TYR	CB-CG-CD2	6.93	125.16	121.00
1	A	154[A]	MET	CG-SD-CE	6.81	111.10	100.20
1	A	154[B]	MET	CG-SD-CE	6.81	111.10	100.20
1	A	463[A]	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	463[B]	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	196[A]	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	196[B]	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	229[A]	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	229[B]	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	463[A]	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	463[B]	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	283[A]	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	283[B]	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	396[A]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	396[B]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	229[A]	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	229[B]	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	303[A]	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	303[B]	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	443[A]	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	443[B]	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	20[A]	TYR	CB-CG-CD1	-5.33	117.81	121.00
1	A	20[B]	TYR	CB-CG-CD1	-5.33	117.81	121.00
1	A	487[A]	PHE	CB-CG-CD1	5.28	124.50	120.80
1	A	487[B]	PHE	CB-CG-CD1	5.28	124.50	120.80
1	A	460[A]	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	460[B]	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	418[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	418[B]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	352[A]	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	352[B]	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	431[A]	ASP	CB-CG-OD1	5.12	122.90	118.30
1	A	431[B]	ASP	CB-CG-OD1	5.12	122.90	118.30
1	A	202[A]	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	202[B]	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	4705	3754	159	0	0
2	A	61	31	0	0	0
3	A	440	0	0	1	0
All	All	5206	3785	159	1	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 1.

All (1) 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)

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	971/510 (190%)	946 (97%)	23 (2%)	2 (0%)	47 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217[A]	VAL
1	A	217[B]	VAL

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	772/407 (190%)	764 (99%)	8 (1%)	76 57

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158[A]	ASN
1	A	158[B]	ASN
1	A	369[A]	LEU
1	A	369[B]	LEU
1	A	432[A]	LEU
1	A	432[B]	LEU
1	A	503[A]	LYS
1	A	503[B]	LYS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.