



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:30 PM EDT

PDB ID : 3MV2
Title : Crystal Structure of a-COP in Complex with e-COP
Authors : Hoelz, A.; Hsia, K.C.
Deposited on : unknown
Resolution : 2.90 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

<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 : **FAILED**
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
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-20030345

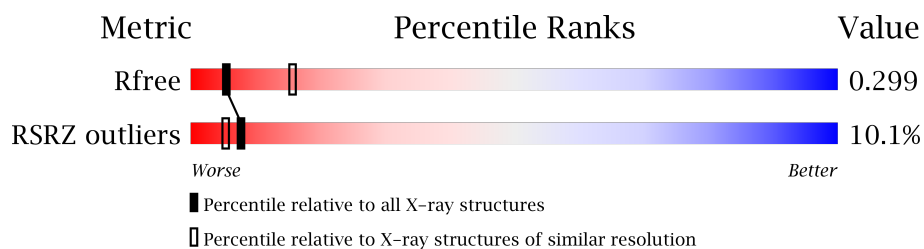
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14273 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2405	1542	403	449	11			
1	C	303	Total	C	N	O	S	0	0	0
			2388	1531	399	447	11			
1	E	303	Total	C	N	O	S	0	0	0
			2388	1531	399	447	11			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP P53622
A	-21	GLY	-	EXPRESSION TAG	UNP P53622
A	-20	SER	-	EXPRESSION TAG	UNP P53622
A	-19	SER	-	EXPRESSION TAG	UNP P53622
A	-18	HIS	-	EXPRESSION TAG	UNP P53622
A	-17	HIS	-	EXPRESSION TAG	UNP P53622
A	-16	HIS	-	EXPRESSION TAG	UNP P53622
A	-15	HIS	-	EXPRESSION TAG	UNP P53622
A	-14	HIS	-	EXPRESSION TAG	UNP P53622
A	-13	HIS	-	EXPRESSION TAG	UNP P53622
A	-12	SER	-	EXPRESSION TAG	UNP P53622
A	-11	SER	-	EXPRESSION TAG	UNP P53622
A	-10	GLY	-	EXPRESSION TAG	UNP P53622
A	-9	LEU	-	EXPRESSION TAG	UNP P53622
A	-8	GLU	-	EXPRESSION TAG	UNP P53622
A	-7	VAL	-	EXPRESSION TAG	UNP P53622
A	-6	LEU	-	EXPRESSION TAG	UNP P53622
A	-5	PHE	-	EXPRESSION TAG	UNP P53622
A	-4	GLN	-	EXPRESSION TAG	UNP P53622
A	-3	GLY	-	EXPRESSION TAG	UNP P53622
A	-2	PRO	-	EXPRESSION TAG	UNP P53622
A	-1	HIS	-	EXPRESSION TAG	UNP P53622
A	0	MET	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MET	-	EXPRESSION TAG	UNP P53622
C	-21	GLY	-	EXPRESSION TAG	UNP P53622
C	-20	SER	-	EXPRESSION TAG	UNP P53622
C	-19	SER	-	EXPRESSION TAG	UNP P53622
C	-18	HIS	-	EXPRESSION TAG	UNP P53622
C	-17	HIS	-	EXPRESSION TAG	UNP P53622
C	-16	HIS	-	EXPRESSION TAG	UNP P53622
C	-15	HIS	-	EXPRESSION TAG	UNP P53622
C	-14	HIS	-	EXPRESSION TAG	UNP P53622
C	-13	HIS	-	EXPRESSION TAG	UNP P53622
C	-12	SER	-	EXPRESSION TAG	UNP P53622
C	-11	SER	-	EXPRESSION TAG	UNP P53622
C	-10	GLY	-	EXPRESSION TAG	UNP P53622
C	-9	LEU	-	EXPRESSION TAG	UNP P53622
C	-8	GLU	-	EXPRESSION TAG	UNP P53622
C	-7	VAL	-	EXPRESSION TAG	UNP P53622
C	-6	LEU	-	EXPRESSION TAG	UNP P53622
C	-5	PHE	-	EXPRESSION TAG	UNP P53622
C	-4	GLN	-	EXPRESSION TAG	UNP P53622
C	-3	GLY	-	EXPRESSION TAG	UNP P53622
C	-2	PRO	-	EXPRESSION TAG	UNP P53622
C	-1	HIS	-	EXPRESSION TAG	UNP P53622
C	0	MET	-	EXPRESSION TAG	UNP P53622
E	-22	MET	-	EXPRESSION TAG	UNP P53622
E	-21	GLY	-	EXPRESSION TAG	UNP P53622
E	-20	SER	-	EXPRESSION TAG	UNP P53622
E	-19	SER	-	EXPRESSION TAG	UNP P53622
E	-18	HIS	-	EXPRESSION TAG	UNP P53622
E	-17	HIS	-	EXPRESSION TAG	UNP P53622
E	-16	HIS	-	EXPRESSION TAG	UNP P53622
E	-15	HIS	-	EXPRESSION TAG	UNP P53622
E	-14	HIS	-	EXPRESSION TAG	UNP P53622
E	-13	HIS	-	EXPRESSION TAG	UNP P53622
E	-12	SER	-	EXPRESSION TAG	UNP P53622
E	-11	SER	-	EXPRESSION TAG	UNP P53622
E	-10	GLY	-	EXPRESSION TAG	UNP P53622
E	-9	LEU	-	EXPRESSION TAG	UNP P53622
E	-8	GLU	-	EXPRESSION TAG	UNP P53622
E	-7	VAL	-	EXPRESSION TAG	UNP P53622
E	-6	LEU	-	EXPRESSION TAG	UNP P53622
E	-5	PHE	-	EXPRESSION TAG	UNP P53622
E	-4	GLN	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P53622
E	-2	PRO	-	EXPRESSION TAG	UNP P53622
E	-1	HIS	-	EXPRESSION TAG	UNP P53622
E	0	MET	-	EXPRESSION TAG	UNP P53622

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			
2	D	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			
2	F	293	Total	C	N	O	S	0	0	0
			2364	1508	371	480	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	EXPRESSION TAG	UNP P40509
B	-12	GLY	-	EXPRESSION TAG	UNP P40509
B	-11	SER	-	EXPRESSION TAG	UNP P40509
B	-10	SER	-	EXPRESSION TAG	UNP P40509
B	-9	HIS	-	EXPRESSION TAG	UNP P40509
B	-8	HIS	-	EXPRESSION TAG	UNP P40509
B	-7	HIS	-	EXPRESSION TAG	UNP P40509
B	-6	HIS	-	EXPRESSION TAG	UNP P40509
B	-5	HIS	-	EXPRESSION TAG	UNP P40509
B	-4	HIS	-	EXPRESSION TAG	UNP P40509
B	-3	SER	-	EXPRESSION TAG	UNP P40509
B	-2	GLN	-	EXPRESSION TAG	UNP P40509
B	-1	ASP	-	EXPRESSION TAG	UNP P40509
B	0	PRO	-	EXPRESSION TAG	UNP P40509
D	-13	MET	-	EXPRESSION TAG	UNP P40509
D	-12	GLY	-	EXPRESSION TAG	UNP P40509
D	-11	SER	-	EXPRESSION TAG	UNP P40509
D	-10	SER	-	EXPRESSION TAG	UNP P40509
D	-9	HIS	-	EXPRESSION TAG	UNP P40509
D	-8	HIS	-	EXPRESSION TAG	UNP P40509
D	-7	HIS	-	EXPRESSION TAG	UNP P40509
D	-6	HIS	-	EXPRESSION TAG	UNP P40509
D	-5	HIS	-	EXPRESSION TAG	UNP P40509
D	-4	HIS	-	EXPRESSION TAG	UNP P40509

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	-	EXPRESSION TAG	UNP P40509
D	-2	GLN	-	EXPRESSION TAG	UNP P40509
D	-1	ASP	-	EXPRESSION TAG	UNP P40509
D	0	PRO	-	EXPRESSION TAG	UNP P40509
F	-13	MET	-	EXPRESSION TAG	UNP P40509
F	-12	GLY	-	EXPRESSION TAG	UNP P40509
F	-11	SER	-	EXPRESSION TAG	UNP P40509
F	-10	SER	-	EXPRESSION TAG	UNP P40509
F	-9	HIS	-	EXPRESSION TAG	UNP P40509
F	-8	HIS	-	EXPRESSION TAG	UNP P40509
F	-7	HIS	-	EXPRESSION TAG	UNP P40509
F	-6	HIS	-	EXPRESSION TAG	UNP P40509
F	-5	HIS	-	EXPRESSION TAG	UNP P40509
F	-4	HIS	-	EXPRESSION TAG	UNP P40509
F	-3	SER	-	EXPRESSION TAG	UNP P40509
F	-2	GLN	-	EXPRESSION TAG	UNP P40509
F	-1	ASP	-	EXPRESSION TAG	UNP P40509
F	0	PRO	-	EXPRESSION TAG	UNP P40509

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3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	329.13Å 74.38Å 97.25Å 90.00° 102.27° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.02 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.4 (20.00-2.90) 85.9 (20.02-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.297 0.246 , 0.299	Depositor DCC
R_{free} test set	1938 reflections (4.43%)	DCC
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14273	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	305/325 (93%)	-0.17	6 (1%) 65 62	55, 89, 144, 199	0
1	C	303/325 (93%)	0.07	15 (4%) 30 25	57, 97, 167, 201	0
1	E	303/325 (93%)	0.84	47 (15%) 2 1	98, 157, 196, 201	0
2	B	293/310 (94%)	-0.00	14 (4%) 31 27	59, 99, 166, 201	0
2	D	293/310 (94%)	0.12	13 (4%) 35 30	64, 104, 172, 201	0
2	F	293/310 (94%)	1.52	85 (29%) 1 0	106, 179, 201, 201	0
All	All	1790/1905 (93%)	0.39	180 (10%) 8 5	55, 119, 197, 201	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	160	ASN	9.2
2	F	29	THR	8.9
2	F	153	GLU	8.8
2	F	51	ASP	8.6
1	C	1135	ASP	7.6
2	F	50	GLN	7.3
2	F	70	LYS	7.3
2	D	155	THR	7.3
2	F	83	GLN	6.9
1	C	1133	ALA	6.6
2	F	257	ASP	6.1
2	F	178	GLU	6.1
2	F	118	ALA	6.1
2	F	180	ALA	6.0
2	F	20	GLN	6.0
2	F	1	MET	5.9
2	F	47	TYR	5.8
1	E	979	GLN	5.8
2	F	58	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
2	D	258	THR	5.7
2	F	116	ASP	5.7
2	F	48	GLN	5.5
2	F	151	ALA	5.4
2	B	29	THR	5.3
1	A	1144	TYR	5.3
2	F	84	ASN	5.1
2	B	156	VAL	4.9
1	E	1057	LEU	4.9
1	E	977	GLU	4.8
1	E	1165	SER	4.7
2	F	27	LYS	4.7
1	E	1135	ASP	4.7
2	F	30	ASP	4.7
2	F	31	ASN	4.7
2	F	143	THR	4.7
2	F	152	ILE	4.6
1	E	1093	HIS	4.5
2	B	154	ASP	4.4
1	C	1060	GLY	4.4
2	D	81	ASP	4.3
1	E	1058	LYS	4.3
2	F	26	SER	4.2
1	E	1144	TYR	4.2
1	E	1196	GLY	4.2
1	E	1124	LYS	4.1
2	F	3	TYR	4.1
2	F	2	ASP	4.1
2	B	155	THR	4.0
2	B	117	GLU	4.0
2	F	107	GLU	3.9
2	F	161	GLU	3.9
2	F	147	ASN	3.8
2	F	15	PHE	3.8
1	E	1055	ARG	3.8
2	D	1	MET	3.8
2	F	53	THR	3.7
1	C	1138	PRO	3.7
1	A	1099	PHE	3.7
2	F	99	LEU	3.7
2	F	233	LYS	3.6
2	F	44	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	1174	VAL	3.6
1	E	1097	LYS	3.6
1	E	1115	SER	3.5
1	A	-2	PRO	3.5
1	C	1058	LYS	3.5
1	C	1059	GLU	3.5
2	F	104	LYS	3.5
2	F	28	VAL	3.5
2	D	26	SER	3.5
1	C	1117	PRO	3.5
1	E	974	THR	3.4
2	F	11	TYR	3.4
1	E	1089	ALA	3.4
2	F	24	LYS	3.4
2	F	179	THR	3.4
1	E	965	LEU	3.3
2	F	52	PRO	3.3
2	D	27	LYS	3.3
1	C	973	ASP	3.2
2	F	177	LYS	3.2
2	F	117	GLU	3.2
1	E	962	PRO	3.2
2	F	91	LEU	3.2
1	E	1146	LYS	3.1
2	B	116	ASP	3.1
1	E	909	LYS	3.1
2	F	121	THR	3.1
2	F	10	TYR	3.1
1	E	1022	LEU	3.1
2	F	46	GLN	3.0
2	F	258	THR	3.0
1	E	1067	GLU	3.0
1	E	963	ALA	3.0
2	F	281	ILE	2.9
2	F	16	VAL	2.9
1	E	1059	GLU	2.9
2	B	27	LYS	2.9
2	F	194	PHE	2.9
2	F	64	VAL	2.8
2	F	159	ASP	2.8
2	F	185	TYR	2.8
2	F	155	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	156	VAL	2.8
2	F	18	CYS	2.8
2	B	26	SER	2.8
1	E	967	TYR	2.8
1	E	1100	LEU	2.8
1	E	1060	GLY	2.8
1	E	1127	ASN	2.8
2	F	112	GLY	2.8
2	F	25	PHE	2.8
1	E	1003	LEU	2.7
2	B	18	CYS	2.7
2	F	129	ILE	2.6
2	D	2	ASP	2.6
2	F	293	ASP	2.6
1	C	1094	PHE	2.6
2	B	118	ALA	2.6
2	F	267	LYS	2.6
2	F	135	ASN	2.6
2	F	287	GLU	2.6
2	F	12	THR	2.5
1	E	1160	ASP	2.5
2	F	268	LEU	2.5
2	D	80	LYS	2.5
2	F	89	LEU	2.5
2	F	148	TYR	2.5
2	F	120	GLY	2.5
1	E	1129	ALA	2.5
1	E	1125	ILE	2.4
2	F	19	LEU	2.4
1	E	1150	CYS	2.4
1	A	1146	LYS	2.4
1	C	974	THR	2.4
2	F	249	THR	2.4
2	F	77	ASN	2.4
2	F	243	PHE	2.3
2	F	88	GLU	2.3
1	E	1172	LYS	2.3
2	D	55	LYS	2.3
1	E	920	PHE	2.3
2	F	145	PHE	2.3
2	F	193	THR	2.3
2	D	70	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	290	ARG	2.3
2	F	211	ARG	2.3
2	F	85	SER	2.2
2	B	28	VAL	2.2
2	D	116	ASP	2.2
1	C	1195	SER	2.2
2	F	274	PHE	2.2
1	C	1131	SER	2.2
1	E	1134	SER	2.2
1	E	1102	ALA	2.1
1	E	1189	LYS	2.1
1	E	1159	GLU	2.1
1	A	1132	MET	2.1
1	E	1095	LYS	2.1
2	B	213	ILE	2.1
2	F	80	LYS	2.1
1	C	1100	LEU	2.1
1	E	953	TYR	2.1
1	E	1120	GLU	2.1
1	C	1164	VAL	2.1
2	F	119	GLU	2.1
2	B	230	VAL	2.1
2	F	87	TYR	2.1
1	A	1129	ALA	2.1
1	E	1145	ALA	2.1
2	F	146	ASP	2.0
2	D	117	GLU	2.0
2	F	69	THR	2.0
2	F	8	GLN	2.0
1	E	1006	PRO	2.0
1	E	948	GLU	2.0
1	E	1194	ALA	2.0
1	E	1062	THR	2.0
1	C	1124	LYS	2.0
2	B	83	GLN	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates

There are no carbohydrates in this entry.

5.4 Ligands

There are no ligands in this entry.

5.5 Other polymers

There are no such residues in this entry.