



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:41 PM EDT

PDB ID : 3MV3
Title : Crystal Structure of a-COP in Complex with e-COP
Authors : Hoelz, A.; Hsia, K.C.
Deposited on : unknown
Resolution : 3.25 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

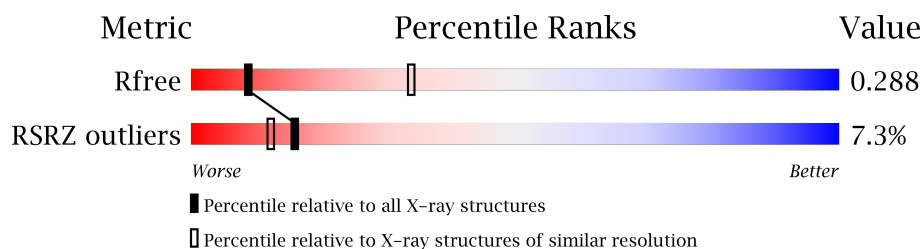
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1852 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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 14256 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	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	C	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	E	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	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	MSE	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MSE	-	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	MSE	-	EXPRESSION TAG	UNP P53622
E	-22	MSE	-	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	MSE	-	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	Se	0	0	0
			2364	1508	371	480	2	3			
2	D	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			
2	F	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MSE	-	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	MSE	-	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	MSE	-	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	328.13Å 74.31Å 96.40Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 48.68 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.7 (50.00-3.25) 96.1 (48.68-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.287 0.250 , 0.288	Depositor DCC
R_{free} test set	1705 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 125.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14256	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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	296/325 (91%)	-0.03	2 (0%) 87 83	47, 89, 147, 193	0
1	C	296/325 (91%)	0.08	3 (1%) 82 76	56, 111, 179, 201	0
1	E	296/325 (91%)	1.15	68 (22%) 1 1	113, 171, 201, 201	0
2	B	290/310 (93%)	-0.03	1 (0%) 93 92	44, 96, 169, 188	0
2	D	290/310 (93%)	0.05	5 (1%) 70 61	59, 110, 173, 201	0
2	F	290/310 (93%)	0.87	49 (16%) 2 1	92, 177, 201, 201	0
All	All	1758/1905 (92%)	0.35	128 (7%) 16 12	44, 127, 196, 201	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1141	PHE	10.0
1	E	1197	LEU	8.5
1	C	1135	ASP	7.5
1	E	1129	ALA	7.0
1	E	1149	ILE	6.5
2	F	160	ASN	6.4
1	E	1139	ILE	6.3
1	E	1133	ALA	5.2
2	F	55	LYS	5.2
1	E	909	LYS	5.0
2	F	227	TYR	5.0
1	E	1140	ASP	4.9
2	F	83	GLN	4.8
1	E	1138	PRO	4.8
2	F	285	PHE	4.8
1	E	1147	PHE	4.7
2	F	89	LEU	4.6
1	E	927	LEU	4.4
1	E	1146	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	911	PRO	4.3
2	F	154	ASP	4.3
1	E	1099	PHE	4.2
1	E	1199	ILE	4.2
1	C	1059	GLU	4.2
1	E	920	PHE	4.2
2	F	187	TYR	4.2
1	E	1154	TYR	4.1
2	F	29	THR	4.0
1	E	1160	ASP	4.0
2	F	179	THR	3.9
2	F	113	ILE	3.9
1	E	1127	ASN	3.9
1	E	1171	SER	3.9
1	E	1142	ASP	3.8
1	E	1155	LYS	3.8
1	E	1044	TYR	3.8
2	F	70	LYS	3.7
2	F	26	SER	3.6
1	E	1135	ASP	3.6
2	F	281	ILE	3.6
2	F	33	LEU	3.5
2	F	32	THR	3.5
1	E	1021	THR	3.5
1	E	1068	LEU	3.5
2	F	25	PHE	3.4
2	D	150	ASN	3.4
1	E	1071	TYR	3.3
2	F	164	LEU	3.3
2	F	75	LEU	3.3
2	F	116	ASP	3.2
2	F	258	THR	3.2
1	E	1080	ILE	3.2
2	F	35	PHE	3.2
1	E	1025	VAL	3.2
1	E	1156	PRO	3.2
1	E	1137	ILE	3.2
1	E	1190	ILE	3.1
1	E	979	GLN	3.1
2	F	81	ASP	3.1
2	F	84	ASN	3.1
1	E	1175	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	11	TYR	3.0
2	F	131	VAL	3.0
1	E	978	ASP	2.9
1	A	1144	TYR	2.9
1	E	981	LEU	2.9
2	D	268	LEU	2.9
1	E	1134	SER	2.8
2	F	24	LYS	2.8
1	E	936	LEU	2.8
1	E	1072	PHE	2.8
1	E	1096	HIS	2.8
1	E	1168	LEU	2.8
2	F	118	ALA	2.8
1	E	1128	LYS	2.7
2	D	81	ASP	2.7
1	E	912	ALA	2.7
2	F	22	ILE	2.7
1	E	938	PRO	2.7
1	E	1059	GLU	2.7
1	E	1174	VAL	2.7
2	F	30	ASP	2.7
1	E	967	TYR	2.7
2	F	34	LEU	2.7
1	E	1048	LEU	2.6
2	F	130	GLU	2.6
2	F	147	ASN	2.6
2	F	178	GLU	2.6
2	F	67	LEU	2.6
1	E	1195	SER	2.6
2	D	258	THR	2.6
2	D	227	TYR	2.6
1	E	1063	VAL	2.6
1	E	1124	LYS	2.5
2	F	7	LYS	2.5
1	E	1031	GLU	2.5
1	E	1153	THR	2.4
2	F	163	ILE	2.4
1	E	923	ALA	2.4
2	F	3	TYR	2.4
1	E	1187	ILE	2.4
1	E	1161	THR	2.4
2	F	60	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	28	VAL	2.4
1	E	1066	LEU	2.4
1	E	1176	THR	2.3
1	E	1067	GLU	2.3
2	F	8	GLN	2.3
2	B	55	LYS	2.3
2	F	124	LEU	2.3
2	F	90	TYR	2.3
1	E	1159	GLU	2.3
1	E	1047	GLY	2.3
1	E	1077	LEU	2.2
2	F	235	ASN	2.2
2	F	144	ILE	2.2
2	F	121	THR	2.2
1	E	1196	GLY	2.2
2	F	274	PHE	2.1
1	E	1150	CYS	2.1
1	E	1125	ILE	2.1
2	F	183	ASN	2.1
2	F	58	LYS	2.1
1	E	1009	ALA	2.1
1	C	935	LYS	2.0
1	A	1128	LYS	2.0
1	E	1094	PHE	2.0
1	E	1070	ALA	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.